A Guide to Using

DynaChem

Version 17.0

(ESP version 9.0)

OLI Systems, Inc

Please note that the example problems in this manual were run under DynaChem Version 17.0 Therefore, due to the ongoing refinement of the underlying OLI Databank, the results produced by your current DynaChem may show modest differences from those shown in this manual.

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PREFACE

DynaChem is the primary dynamic simulation component of the ProChem (Program for Chemical Simulation) System. Specifically, DynaChem allows for description of one or more process units which are physically tied together by processing streams and, where applicable, process control. The entire system is solved on an unsteady-state (time-dependent) basis.

DynaChem is supported by a thermodynamic framework and associated databank which allows a User to call upon a broad spectrum of reactive chemistry and reactive phenomena. The architecture of the program is such that the User need know only the names of the chemicals involved and not the detailed chemical reactions.

Chapter 1: Introduction

Philosophy

The philosophy of DynaChem is based upon discrete, modular computation of "process" units. The term process is a general term in this case referring to any chemical system. This can range from a traditional chemical process to a geological system being altered by the environment.

The concept of isolating a process unit as a discrete computation allows for the assumption of homogeneity and chemical and thermodynamic equilibrium. However, limits to homogeneity and equilibrium may be established by allowing for imperfect mixing and an approach to equilibrium. Once a process has been identified as a series of discrete units, a two-tier "stepping" technique is employed to simulate the dynamic nature of the process.

The first tier (inner tier) steps through the units in a predefined order for specified time increment. The order typically begins with mass/energy flow into the process and ends with mass/energy flow out of the process. The ordering, however, is flexible and may be altered to achieve special process conditions such as recycle.

In the stepping from one unit to the next unit in order, "packets" of mass/energy are introduced into the unit, mixed, and the resulting equilibrium condition is determined. At this point, limits to mixing (homogeneity) and equilibrium may be introduced by such principles as mixing dynamics and reaction kinetics. The outgoing packets are then determined by specified parameters such as tank level, valve opening and fluid pressure. The outgoing packets of mass/energy are then passed to the next unit in order and the procedure is repeated for that unit.

This first tier of computation should be conceptualized as the movement of mass/energy through a process during a small but finite increment of time.

The second tier (outer tier) uses the final state of the process as defined by the inner tier as the beginning state for the next time increment. The outer tier "steps" through time, with each step resulting in a complete pass through the inner tier.

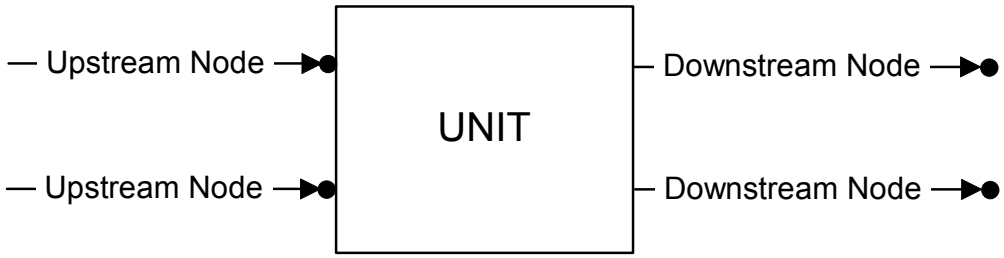
The discrete nature of the computation allows for a high level of flexibility in adding computation definition before the simulation is performed and altering of system parameters during simulation.

Structure

The structure of DynaChem is based upon Units and Nodes.

As described in the DynaChem Philosophy, a Unit is any portion of a process which can be isolated based upon homogeneity and equilibrium. This may include entities such as a tank or a section of pipe, but also may be a schedule of inflows to a process which may be defined as mass/energy flow as a function of time.

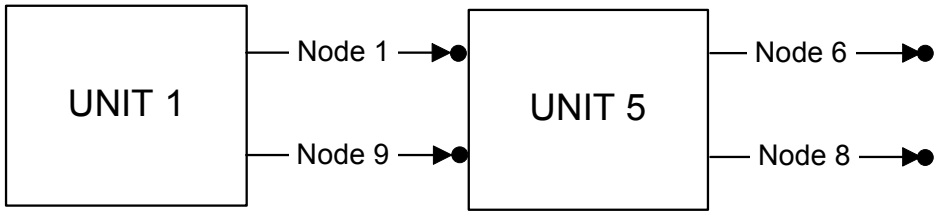
During a defined increment of time "packets" of mass/energy are introduced into a Unit. The mass/energy is combined with the mass/energy already present in the Unit and the equilibrium condition is determined. Based upon defined Unit parameters, "packets" of outgoing mass/energy are determined and placed at collecting points called Nodes.



Thus, the transmission of mass/energy from one Unit to another Unit during a discrete increment of time is by accepting "packets" of mass/energy from Upstream Nodes and depositing "packets" of mass/energy at Downstream Nodes.

This structure of Units and Nodes is established by the User in DynaChem Input. Units and Nodes are numbered and subsequently identified by Unit Number and Node Number.

The computation order of the inner tier (described in Philosophy) is defined by Node Order. Specification of a Node in the computation order results in the execution of the Unit computation for which that Node is a Downstream Node.



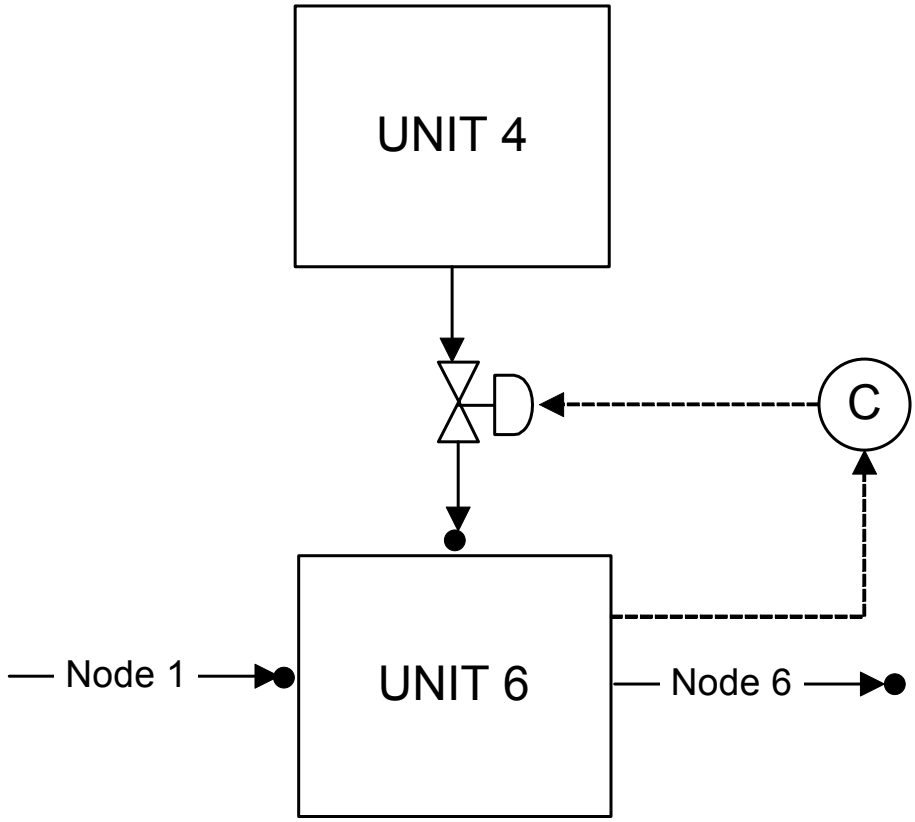
Node Order = 6,9

In the above diagram since the User has specified Node 6 as first in the Node Order, Unit 5 will be computed first, employing as inflows the "packets" placed at Nodes I and 9 during the previous time increment. Outflow packets will be placed at Nodes 6 and 8. Unit 1 will be computed next since Node 9 is second in the Node Order. Packets of mass/energy will be placed at Nodes 1 and 9.

Notice that it is unnecessary, although not prohibited, to include Nodes 8 and 1 in the Node Order. They will necessarily be computed when Unit 5 and Unit 1, respectively, are computed.

The sequence defined by this Node Order may or may not be the best computation order for the process. Nodes 1 and 9 may be considered to be one time step out of phase. There are conditions (e.g., recycle) in which this sequence will be appropriate.

It behooves the User of DynaChem to understand the dynamics of the process before establishing the Unit definition and Node computation order. Implicit dead time may be introduced by manipulation of the Node Order. For example, in the following process illustrated in the diagram below, the packet placed at Node 4 will depend upon the state of Unit 6 because of the control loop. The Node Order of 6,4 will result in no dead time since the state of Unit 6 will be determined for the time increment before the control loop linked to Unit 4 is computed. The Node Order of 4,6 will result in dead time equal to one time increment because Unit 4 will be computed first, using the state of Unit 6 at completion of the previous time increment.



The Unit and Node structure and Node Order defined by the user provides flexibility but must be carefully examined to achieve the desired results.

Unit Specification

There are three types of Units available in DynaChem. They are named (1) ENTRY, (2) TANK and (3) PIPE.

The ENTRY Unit provides a means of introducing mass/energy into the process by continuous flow, intermittent flow or scheduled flow. The mass/energy flow may be defined by direct input or based upon values saved from a previous DynaChem execution.

The TANK Unit may be used for any vessel or collection of mass/energy which may change in quantity and/or volume as well as state. In many cases this will be a tank, but also may be the shell side of a boiler, a tray of a distillation column or a continuous stirred-tank reactor (CSTR). The TANK is defined physically by cross-sectional area, maximum level, maximum volume and exit level. The liquid level is computed and updated every time increment.

The PIPE Unit may be used for any process unit which maintains constant volume. This may be no more than a section of pipe, but may also be the tube side of a heat exchanger, a heating or cooling coil or a plug flow reactor (PFR).

The PIPE is physically defined by cross-sectional area, length and maximum volume. Level is not applicable to PIPE Units. No mass may exit a PIPE until the volume is fun. Mass enters the PIPE and sufficient mass exits to maintain the full volume of the PIPE.

Many dynamic systems may be modeled with DynaChem using nothing more than Units and Nodes. For such systems, no further description of Valves, Pumps and Control Loops is necessary.

Most processes, however, require some use of these attributes to model the precise operation of the process components.

Valve Specifications

A VALVE is used to restrict the flow of mass/energy and, therefore, the amount of mass/energy which may be placed at a Node, during a time increment. The placement of a VALVE is defined by its downstream Node (DNODE).

The maximum flow is set by the Valve capacity and the actual flow is determined by the Valve Stem Position (fraction open). The Step Position may be set by the User (manual) or by a Control Loop (automatic).

Alternate VALVE types are available.

Pump Specification

A PUMP is used to increase the fluid pressure. The placement of a PUMP is defined by the

downstream Node **(DNODE).**

The discharge pressure of a pump is computed from the suction pressure and the Head developed by the pump. The Head is determined from a pump curve (entered by the User) as a function of flow and pump speed.

Control Loop Specification

In general, a Control Loop (1) measures a process variable (temperature, pressure, pH, level, flow or composition) from a specified Unit or Node (i.e., "stream"), (2) compares that value to a specified Setpoint and, as a result, (3) makes adjustments to a Valve (Stem Position), a Pump (Speed) or another Control Loop (Setpoint).

Various controller algorithms are available including Velocity, Positional, Switch, Multicascade, Ratio and Trim. For PID controllers, the Gain, Integral time and Derivative time are selected by the User but may be changed during execution for "tuning" purposes. Dead Time, Controller output limits and Controller output factors may be specified.

Time, Print and Save Specifications

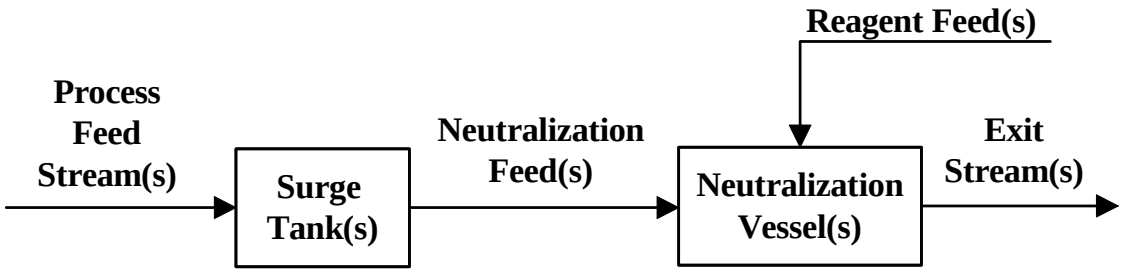
The Time Increment and End Time must be specified for all executions.

The PRINT specification is used to set the frequency of printing (to computer files) of output, summary and "trace" information. The PRINT specification is also used to set the mode to Interactive if desired.

The SAVE specification is used to set the frequency of saving the Restart file**.** It is also used to save Node information for the LOGNODE capability.

Chapter 2: Building a DynaChem Case

Building a DynaChem Case is accomplished in much the same manner as building a steady-state process simulation case. First, the process should be sketched with the appropriate inflows, process units and connecting streams. Conversion to dynamic units should not be attempted until the basic layout is complete. For example, a simple neutralization process may be represented as shown below:

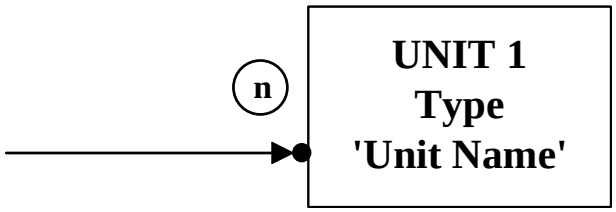


Process control, valves, pumps and auxiliary units may be added after the basic units have been specified.

Unit Definition

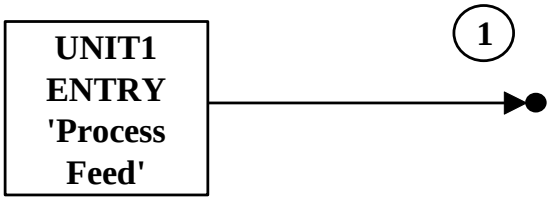
The Process Feed Stream should be defined first. Since there are no upstream units to define the now at this point, a DynaChem ENTRY Unit must be used.

Before describing the DynaChem Input, however, a note about nomenclature is in order. In the following discussion, Units will be designated with a box:



and Nodes will be designated with a line terminated with an arrowhead and termination point, noted with a circle containing the Node Number.

In the case of the Process Feed Stream, the Unit will be Unit 1 and the resulting feed stream will accumulate at Node 1.



The identifying numbers for Units and Nodes are arbitrary and may be any integer from 1 to 50. In this case, the Node Number is the same as the Unit Number for convenience only. The Downstream Node Number need not be the same as the Unit Number.

The Unit and Downstream Node have been identified. Now, the Unit should be defined, beginning with the State of the stream. This includes temperature, pressure, flow and composition. Since this is an ENTRY Unit and is used to define flow, the one extensive property (flow) is time dependent (m^3/hr) and we refer to the "State of the stream." The TANK and PIPE Units define physical Units which accumulate mass. In these Units, the extensive property is the volume of fluid contained in the Unit (m^3) and we refer to the "State of the contents." In either case, State defines the thermochemical conditions of the fluid being defined by the Unit

Entry Unit Definition

In defining the ENTRY, the flow may be continuous, intermittent or scheduled. It is necessary to know the time at which the flow begins, the time over which it builds to maximum flow and the duration of the flow. (Later, a valve may be added to adjust the maximum flow.) In this case, we will initiate the flow at the beginning of the simulation, allow 0.05 hours to reach fun flow (Ramp time = 0.05 hour) and allow the flow to continue indefinitely (continuous flow). The State of the Process Feed Stream will be as follows:

Temperature, Pressure: 250 °C, 1 atm

Maximum Flow Rate: 40 m^3/hr

Composition (in the order of the Chemistry Model Generation (Generate) Output):

H20	55.51 gmole
NAN03	0.01
HN03	0.75
NAOH	0.0
NA2CO3	0.04

The composition of 55.51 gmoles of H20, 0.01 gmole of NaNO3, etc., are "relative" quantities. Values of 1.0, 0.00018, etc., are equivalent since the relative molar quantities are the same. The total mass is determined by the Flow Rate. Composition determines only the relative molar quantities.

The DynaChem Input for this Unit may now be assembled. All DynaChem input must begin with a Primary Keyword (See Reference Table 1). In this case, the Primary Keyword is UNIT.

Primary Keywords are followed by Specification Keywords (See Reference Tables 2 and 3) which apply to the Primary Keyword in effect until another Primary Keyword is employed.

The flow characteristics are translated into DynaChem Input using Specification Keywords as follows:

STATE	=	Temperature (°C), Pressure (atm), Maximum Flow Rate (m^3/hr), Composition in order of the Inflow List as specified in the Generate Output. The composition may be in any units, as long as they are entered in relative molar amounts.
INITIATE	=	Initiation time (hr)
TRAMP	=	Ramp time (hr)
DURATION	=	Duration (hr)
'Name'	=	Unit Name

The Primary and Specification Keywords are then assembled to create the definition of Unit 1:

```
UNIT1 ENTRY DNODE=L INITIATE=0
      TRAMP=0.05 DURATION=0
      'PROCESS FEED'
      STATE = 25, 1, 40, 55-51, 0.01, 0.75, 0,0.4
```

The series of Specification Keywords must be initiated with a Primary Keyword. In the case of UNIT, its Identification Number must also be included. The Specification Keywords should be

1) in any order,
2) separated from each other by at least one space,
3) placed on multiple lines if desired,
4) continued on a subsequent line with a "+" in column 1 (This applies to continuation of the entries pertaining to a single Specification Keyword. Starting a subsequent line with a Specification Keyword is not considered a continuation.)

In many cases there are default values for Specification Keywords (See Reference Table 3), in which case the entry may be omitted. For example, the default for the initiation of an ENTRY flow is zero (INITIATE=0) and the default for duration is continuous (DURATTON=0). Therefore, the above Input may be amended to

```
UNIT1     ENTRY  DNODE=L  TRANP=0.05  'PROCESS FEED'
          STATE=25, 1, 40, 55.51, 0.01, 0.75, 0, 0.04
```

Defining Tank Units

The Process Feed Stream is now defined. The next Unit in the Process is the Surge Tank, the destination of the Process Feed. The Surge Tank is characterized by a TANK with varying volume and state conditions. First, the physical characteristics of the tank must be defined. This is accomplished by defining two of the three following parameters:

1) Cross-section area (CSA)

2) Maximum level

3) Maximum volume

In our case, we will define the CSA and maximum level. The maximum volume is thus implied as

Maximum Volume = Maximum Level * CSA

The Surge Tank will have a CSA of 7.07 m^2 (radius 1.5 m) with a maximum level of 6 m. The maximum volume is, therefore, 42.4 m^3.

Likewise, the level of the fluid (liquid + solid) is defined as

Level of Fluid = Volume of Fluid / CSA

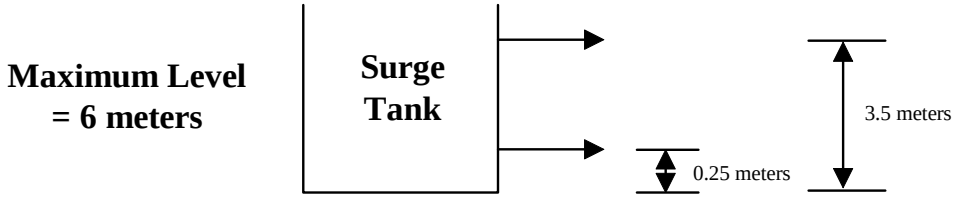
Defining the Surge Tank

The stream, or streams, exiting the tank will be defined by the level at which it exits and its termination Node. The Surge Tank will be Unit 2 and two lines will exit at levels 0.25 m and 3.5 m. The lower exit will be the primary process flow and the higher level will provide overflow capability.

Fluid may flow through an exit only if the fluid is at or above the level at which the exit is placed. Furthermore, the fluid (liquid + solid) flows preferentially from the lowest exit to the highest exit. If, during a time period, the level reaches a height above the higher exit, but sufficient fluid exits the lower exit to reduce the level below the upper exit, then no fluid exits the higher exit. If, however, the fluid removed from the lower exit does not lower the level below the upper exit, then fluid flows out both exits.

Vapor exits preferentially from the highest exit to the lowest exit. However, vapor may not flow through an exit which is below the fluid (liquid + solid) level.

A diagram of the Surge Tank is as follows:



CSA = 7.07 square meters

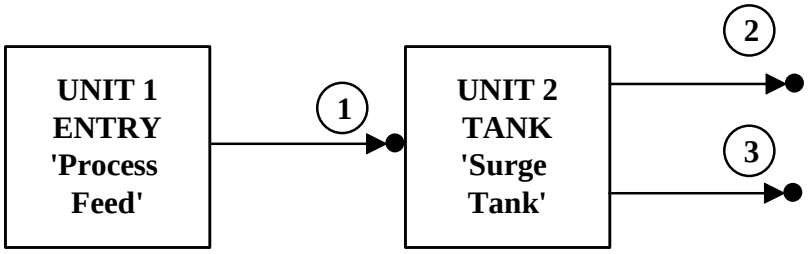
This defines the physical characteristics of the tank itself. The outlet lines will terminate with Node 2 (0.25m) and Node 3 (3.5 m). The initial State of the fluid contained in the tank will be defined as 20 m^3 of pure water at 20°C.

Temperature, Pressure: 20°C, 1 atm

Initial Liquid: 20 m^3

Composition: H20 1.0

The previously defined Feed Stream (Unit 1) provides the Upstream Node. The DynaChem diagram becomes:



The DynaChem Input for the Surge Tank:

```
UNIT2 TANK UNODE=1 DNODE=2,3 LEXIT=0.25,3.5
      'SURGE TANK' CSA=7.07 MAXLEVEL=6
      STATE=20,1,20,1
```

Defining the Neutralization Tank

It should be noted that to this point we have described only the physical characteristics of the Surge Tank, its exits, and the initial contents of the tank. The flow through the exit lines will be further determined by the valves in those lines (capacity and fraction open) and the fluid pressure determined by liquid height and pump (flow and speed). These parameters may in turn be determined by Control Loops. All of these will be described later.

The next Unit is the Neutralization Tank, the Unit in which the neutralization takes place. The Neutralization Tank is defined similarly to the Surge Tank. It has a CSA of 3.14 m' (radius = 1 m) and a maximum level of 4 m. The fluid will exit the Neutralization Tank flowing over the overflow baffle at the maximum level of 4 m. Thus, all fluid above that level will exit. The tank will be Unit 3 and the exit will be to Node 6. The initial contents will be 5.5 m' of pure water at 200.

The DynaChem Input for the Neutralization Tank:

```
UNIT3 TANK UNODE=2,5 DNODE=6 LEXIT=4
      'NEUTRALIZATION TANK'
      CSA=3.14 MAXLEVEL=4 STATE=20,1,5.5,1
```

The final unit in the Neutralization Process is the Reagent Feed. This may be represented as a tank with specified contents or merely as an ENTRY feed stream. For this case, the latter approach will be used. The Reagent flow will be 20 weight % NAOH (NAOHN is the 4th Inflow) at 20° with a maximum flow of 5 m^3/hour. The flow will be metered with a valve and control loop to be added later. The State of the stream is

Temperature, Pressure: 20°C, 1 atm

Maximum Flow Rate: 5 m^3/hr

Composition (in the order of the Generate Output):

H20	0.8988 gmole
NAN03	0.0
HN03	0.0
NAOH	0.1012
NA2CO3	0.0

The Unit will be Number 4 and the flow at Node 5 and the DynaChem Input for the Reagent

Feed is as follows:

```
UNIT4 ENTRY DNODE=5 ‘REAGENT FEED’
              STAT'E = 20, 1, 5, 0.8988, 0, 0, 0.1012
```

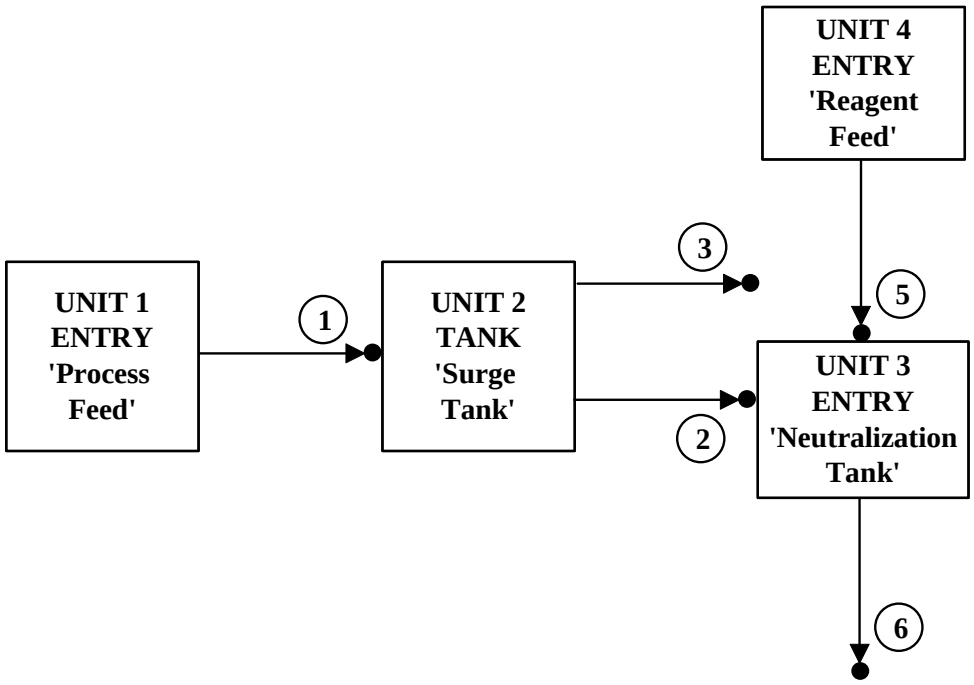
Unit Summary

In summary, the four DynaChem Units are defined as follows:

The DynaChem Input:

```
UNIT1 ENTRY DNODE=1 TRAMP=0.05 ‘PROCESS FEED’
              STATE = 25, 1, 10, 55.51, 0.01, 0.75, 0, 0.04
UNIT2 TANK UNODE=L DNODE=2,3 LEXIT=0.25,3.5
              'SURGE TANK' CSA=7.07 MAXLEVEL=6
              STATE=20,1,20,1
UNIT3 TANK UNODE=2,5 DNODE=6 LEXIT=4
              'NEUTRALIZATION TANK'
              CSA=3.14 MAXLEVEL=4 STATE=20,1,5.5,1
UNIT4         ENTRY DNODE=5 'REAGENT FEED'
```

STATE =20, 1, 5, 0.8988, 0, 0, 0.1012



Valve and Control Loop Definition

Now valves and control loops should be added to achieve the desired process operation. For simplicity, the valves and control loops will be described in the same order as the Units were described.

The exit from Unit 1 (Node 1) does not need a valve. This is a Process Feed which must flow to the Surge Tank. The exits from Unit 2 (Nodes 2 and 3) must be controlled, however, with the following objectives:

1) Maintain the Surge Tank level within acceptable limits

2) Dampen the flow and composition fluctuations to the Neutralization Tank resulting from the intermittent Process Feed Stream. (The fluctuations in this example are not as significant as they are in many neutralization cases in which many streams of different total flow and chemical makeup flow into the Surge Tank.)

On the lower exit (Node 2), at a level of 0.25 m, a valve and deadband level controller will be used to achieve both of these objectives, but primarily objective 2. A valve and level controller on the higher exit (Node 3) will be used as an emergency overflow to complete objective 1.

First, the valve on Node 2 will be identified as Valve 1 (VALV1) and the control loop will be identified as Control Loop 1 (CLO01). Both VALV and CLOO are Primary Keywords (See

Reference Table 1) abbreviated to four letters and will begin DynaChem Input lines. Specification Keywords (See Reference Tables 2 and 3) will be used to specify valve and control parameters.

Valve 1 will have a capacity (C_v) of 40 m^3/hr and will be closed initially (VOPEN=0). The DynaChem Input for Valve 1 is as follows:

VALV1 DNODE=2 CV=40 VOPEN=0

The default for the initial valve stem position is closed. Therefore, VOPEN=0 may be omitted.

To dampen the fluctuations in flow, the controller will use deadband control on the measured Surge Tank level (Unit 2). Deadband control establishes limits between which the measured value (level) is assumed to be equal to the setpoint and, thus, the controller error is zero. When the error is zero, the controller output does not change and, in this case, the valve stem position on the exit to Node 2 does not change. Thus, when the tank level is within the deadband limits (in this case, 1 m to 3 m), the flow to the Neutralization Tank is constant, facilitating pH Control.

If, however, the level does go below the lower limit, the valve is closed under PID Control (Kc=0.2) and, if the level goes above the upper limit, the valve is opened under the same PID Control. Thus, the tank level is maintained. A positive value was chosen for the Gain (Kc) because the controller is to be Direct Acting. That is, when the Error is positive

Error = Measured Variable = Setpoint

then the valve should increase its opening. To increase its opening the Valve Step Position must increase

Stem Position change = Kc * Error

Thus, for a positive Error to increase the Step Position, Kc must be positive. In this case, when the level increases above the Setpoint (the Error becomes positive) greater flow is desired (increased Stem Position) to lower the tank level. When the Error is negative (level lower than the Setpoint), the Stem Position decreases, decreasing the flow and causing the level to rise.

Deadband control should be used with the Positional Algorithm only and a Valve Constant (valve stem position when Error=0; also referred to as Bias) must be specified. In this case, a Valve Constant of 0.35 will be specified (VCONSTANT=O.35). That is, when the Surge Tank level is between 1 and 3 m, the valve stem will always be 35% open. Thus, the control loop which will control Valve 1 will have the following characteristics:

Valve to be controlled: Valve 1

Setpoint Unit (Origin of Measured Variable): Unit 2, Level

Deadband Control Limits = 1 m to 3 m

PID Control: Gain (Kc) = 0.2

Positional Algorithm (Bias = 0.35)

The DynaChem Input for Control Loop 1 is as follows:

```
CLOO1 VIID=1 POSITIONAL SPUNIT=2 SPID=LEVEL
      SPVAL=1,3 KC=0.2 VCONSTANT=0.35
```

In neutralization processes, large unexpected Feed Steams can occur causing significant upsets in the process. The deadband controller protects the Neutralization Tank from upsets. To guard against a Surge Tank overflow, however, the upper exit (Node 3), at a level of 3.5 m, is used as a backup exit with the level cannot be effectively maintained by Control Loop 1. The Setpoint of the Controller will be at 4.5 m to prevent the level reaching the maximum of 6 m.

The valve will be identified as Valve 2 (VALV2) and the level control loop will be identified as Control Loop 2 (CLOO2). The Valve will have a capacity of 50 m^3/hr and will be closed initially (which is the default).

```
VALV2 DNODE=3 CV=50
```

The control loop will be a Direct Acting PID Controller with the following characteristics:

Valve to be controlled: Valve 2

Setpoint Unit (Origin of Measured Variable): Unit 2, Level

Setpoint: 4.5 m

PID Control: Gain (Kc) = 0.5

Velocity Algorithm (default)

The DynaChem Input for Control Loop 2 is as follows:

```
CLOO2 VID=2 SPUNIT=2 SPID=LEVEL SPVAL=4.5
      KC=0.5
```

The final control loop will be designed to maintain a constant pH of 9 in the Neutralization Tank. A valve (VALV3) will be placed on the Reagent Feed (Node 5) to adjust the flow of NaOH solution into the Neutralization Tank. The valve will have a capacity of 10 m^3/hr and will be closed initially.

```
VALV3 DNODE=5 CV=10
```

The stem position of Valve 3 will be controlled by Control Loop 3 (CLO03) which measures the pH in the Neutralization Tank (Unit 3), comparing it to the Setpoint of 9.0. The control loop will be a Reverse Acting PID Controller with a Gain of -0.01 and Integral Time of 1 minute. This controller is Reverse Acting because as the pH increases above the Setpoint of 9 (the Error becomes positive) it is necessary to decrease the flow of NaOH solution (decrease the Stem Position). The control loop will have the following characteristics:

Valve to be controlled: Valve 3

Setpoint Unit (Origin of Measured Variable): Unit 3, pH

Setpoint: pH = 9

PM Control: Gain (Kc) = -0.01

Integral Time (TauI) = 1 min

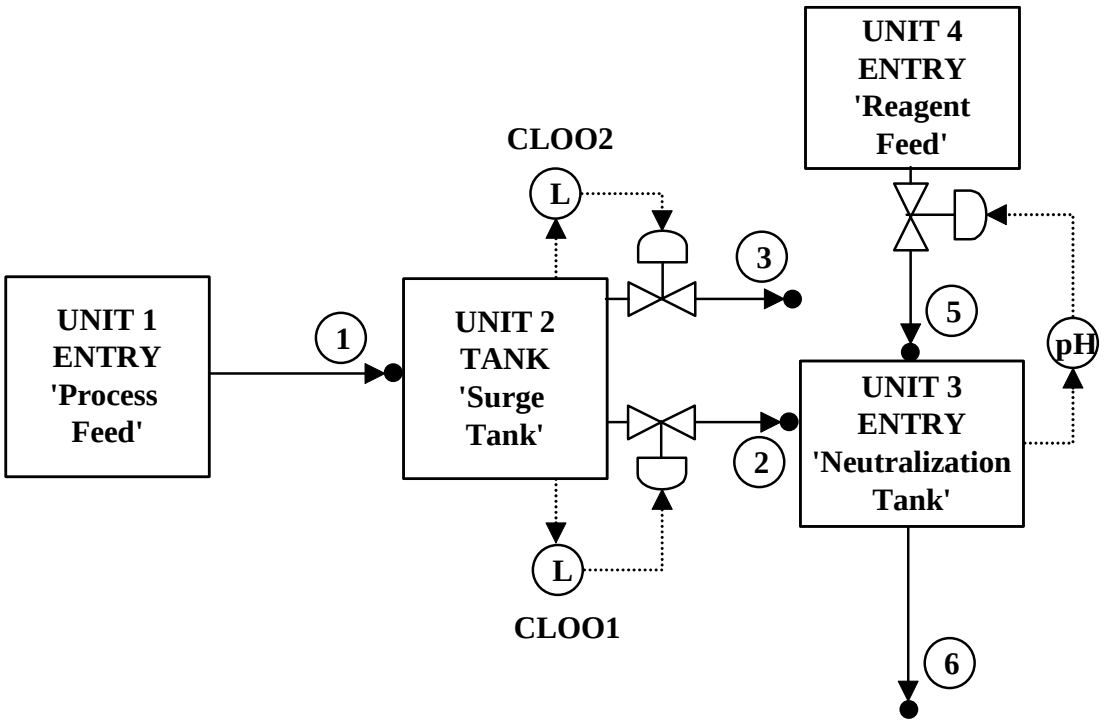
Velocity Algorithm (default)

The DynaChem Input for Control Loop 3 is as follows:

CLOO3 VID=3 SPUNIT=3 SPID=PH SPVAL=9

KC= -0.0l TAUI=1

With the three Control Loops, the Neutralization Process is defined as follows:



The DynaChem Input:

UNIT1 ENTRY DNODE=1 TRAMP=0.05 ‘PROCESS FEED’

STATE = 25, 1, 40, 55.51, 0.01,O.75, 0, 0.04

UNIT2 TANK UNODE=1 DNODE=2,3 LEXIT=0.25, 3.5

‘SURGE TANK’ CSA=7.07 MAXLEVEL=6 STATE=20,1,20,1

```
UNIT3 TANK UNODE=2,5 DNODE=6 LEXIT=4
      ‘     NEUTRALIZANON TANK’
            CSA=3.14 MAXLEVEL=4 STATE=20,1,5.5,1
UNIT4       ENTRY DNODE=5 ‘REAGENT FEED’
            STATE=10,1,5,0.8988,0,0,0.1012
VALV1       DNODE=2 CV=40
VALV2       DNODE=3 CV=50
VALV3       DNODE=5 CV=10
CLOO1       VID=1 POSITIONAL SPUNIT=2 SPID=LEVEL
            SPVAL=1,3  KC=0.2 VCONSTANT=0.35
CLOO2       VID=2 SPUNIT=2 SPID=LEVEL SPVAL=4.5
            KC=0.5
CLOO3   VID=3 SPUNIT=3 SPID=PH SPVAL=9
            KC= -0.0l TAUI=1
```

Time and Node Order Definition

To complete the basic definition of the model, the Time Parameters and Node Order must be specified:

The simulation will be for 1 hour (TEND=l) at time increments of 0.01 hour (TINC=0.01):

```
TIME  TEND=1  TINC=0.0l
```

The objective of DynaChem is to represent an "analog" process with a "digital" and, therefore, discrete model. The time increment is the means of placing the discrete characteristics. The smaller the time increment, the closer the discrete model approaches the analog process. The smaller the time increment, however, the greater the computer time necessary to simulate a given time period. Thus, a compromise between minimizing the departure from analog characteristics and realistic computer execution time is necessary.

In this case, the time increment was selected by trial and error. The time increment was decreased until no significant difference was observed in the System response.

Specification of Node Order determines the order in which all computations are completed. Specification of a Node results in the computation of the following:

1) The Unit directly upstream from the Node (i.e., the Unit for which the Node is a DNODE entry)
2) All Nodes in the DNODE list for that Unit

3) All Valves associated with all Nodes in (2)

4) All Pumps associated with the Valves in (3)

5) All Control Loops associated with the Valves in (3)

6) All Control Loops associated with Control Loops in (5)

Thus, specification of a Node in the Node Order results in the computation of all associated Units, Valves, Pumps and Control Loops.

The Node Order is relatively straightforward in this model. Node 1 will be computed first, resulting in computation of Unit 1. Node 2 will be specified as the second Node. This results in Unit 2 being computed and, therefore, Node 3 as well. Thus, Node 3 need not appear in the Node Order. Node 2 also causes Valves 1 and 2, and Control Loops 1 and 2 to be computed.

Because of Control Loop 3, the order of computation of Nodes 5 and 6 could result in Implicit Dead Time. If Node 6 and, therefore, Unit 3 is computed first, then when Node 5 is computed the pH of Unit 3 for the current time increment will be available to Control Loop 3. In this case, there is no Implicit Dead Time in the control loop since the measured variable is known for the current time and is applied in the control algorithm. If, however, Node 5 is computed first, then the Control Loop 3 is computed before Unit 3 has been computed for the cur-rent time increment. Therefore, the measured variable accessed by the control loop is the value from the previous time increment. The time between measurement of the pH and its use in the control algorithm is one time increment. Therefore, the Implicit Dead Time is equivalent to one time increment.

Since no dead time is desired in this case, Node 6 will be computed before Node 5:

NODE ORDER=1,2,6,5

Summary

This example was not intended to be exhaustive in describing the capabilities or use of DynaChem. Rather, "Building a DynaChem Model" is meant as an example of the procedure which should be used in defining a DynaChem model.

Many other applications of the Units, Valves, Pumps and Control Loops are possible and should be investigated in the appropriate Sections of this Handbook. For details on each of the areas described in the example, you should also refer to the appropriate Sections of Handbook.

Chapter 3: Unit Specification

A Unit is any portion of a process which can be isolated based upon homogeneity and equilibrium.

The Primary Keyword is

UNITi

where i represents a unique identification number from 1 to 50.

There are three types of Units available in DynaChem:

1) ENTRY Unit - introduction of mass and energy into the process
2) TANK Unit - any vessel of collection of mass and energy which may change in quantity and/or volume
3) PIPE Unit - any process unit which maintains constant volume

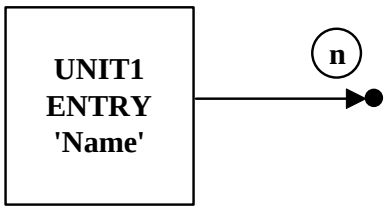
Entry Unit

The ENTRY Unit provides a means of introducing mass and energy into the process by

1) Continuous flow
2) Intermittent flow
3) Scheduled flow (see LOGNODE Capability)

The flow may (1) begin as a step change or (2) be “ramped” from zero to a maximum flow over a specified time period. The maximum flow may be adjusted with a valve which may be controlled by a control loop. Aqueous or non-aqueous streams may be introduced into' the process.

Schematic:



Entry Specifications

Specifications (Required):

DNODE=n	Downstream Node Number - minimum and maximum for Entry Unit is 1
STATE=	T,P,Flow,xl,x2.... State of Entry Stream fluid (Not required when using LOGNODE) Order of entry: Temperature (°C) Pressure (atm) Maximum flow (m^3/hr or Alternate Units) Alternate Flow Units: To enter alternate units, the numeric entry should be followed by (GRAM) for grams/hr or (GMOL) for gmoles/hr. Molar fraction, Inlet Comp 1 Molar fraction, Inlet Comp 2 . . . . Molar fraction, Inlet Comp N
Specifications (Optional):	
INITIATE = til,ti2,...	Time at which Entry flow begins (hr). (default = 0)
DURATION = tdl,td2....	Duration over which Entry flow continues (hr) - zero implies continuous flow. (default=0)
TRAMP = trl,tr2,...	Time during which Entry flow "ramps" from zero flow to maximum flow (hr) - zero implies step change. (default=0)
REPEAT = v,...	Time(s) at which entire series of INITIATE, DURATION, entries are to be repeated. The series to be repeated starts at time=0 and extends through the last INITIATE+DURAT'ION.
LOGNODE = nl,n2....	The Entry flow is to be "Scheduled" by acquiring the Node flows from the Node Input file which was the result of a previous run with SAVE LOGN=nl,n2....

Non-Standard Phase

Nonstandard stream, phase designation. When this designation is used, the Entry stream may be composed of any inflow species in the Chemistry Model. The stream does not need to contain water. Equilibrium condition is not computed, it is defined by the Phase Designation. The enthalpy is computed to make it consistent with any aqueous fluid to which it is added. Density is computed to define flow rate.

Phase =LIQ for liquid (default)

=VAP for vapor

=SOL for solid

Note: When using Nonstandard, the designated phase does NOT need to be present in the Chemistry Model. For example, to inject stream, NONS=VAP may be used even if H20VAP is not in the model. However, in these cases, the DENS and ENTH keywords must be used to specify density an enthalpy.

DENSITY=A,B,C,D Density Coefficients used to compute density of Nonstandard Streams when the chemistry model database does not contain adequate density data.

Density (gmole/liter) = A + B*TK + C*TK**2 + D/TK

TK = Temperature (Kelvin)

ENTHALPY Enthalpy Coefficients used to compute enthalpy of Nonstandard Streams when the chemistry model database does not contain adequate enthalpy data. Enthalpy (cal/gmole) = A + B*TK + C*TK**2 + D/TK

TK = Temperature (Kelvin)

NOVAP Do not allow a vapor phase to be considered. (default = vapor allowed if vapor phase was present in Chemistry Model Definition)

'aaaa' Unit name

Specification Notes

INITIATE, DURATION, TRAMP entries should be matched. That is, Til, tdl, trl represent the first flow interval; ti2, td2, tr2 represent the second; and so on.

Trailing zeros do not need to be entered. Furthermore, if all entries for any one of the Keywords INITIATE, DURATION or TRAMP are zero, then the Keyword itself may be omitted. For example, if all flows are to be step changes, then the Keyword need not be used for the Unit.

Multiple sets of INITIATE, DURATION, TRANP entries must not overlap in time. That is, the first set enters from til to til+tdl. The second set enters from ti2 to ti2+td2. Therefore, ti2 must be greater than or equal to til+tdl.

The maximum number of INITIATE, DURATION, TRAMP sets allowed for ALL ENTRY Units combined is 200. 200 may be entered for a single ENTRY Unit or they may be distributed among the maximum 50 ENTRY Units.

INITIATE, DURATION and TRAMP are not applicable when using LOGNODE.

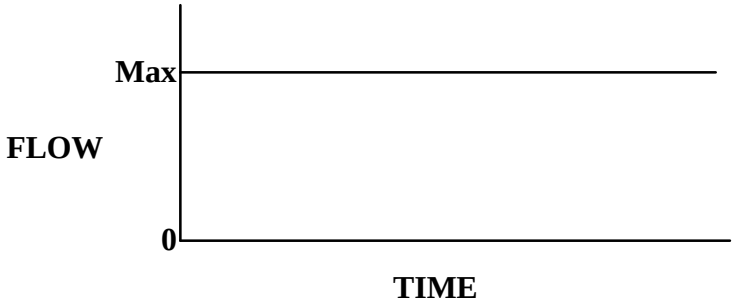
Various flow patterns can be produced with the INITIATE, DURATION and TRAMP Keywords. Continuous flow requires a minimum of Input while Intermittent flow requires a little more specification. However, the REPEAT Keyword may be used to simplify the intermittent characteristics of the Input.

Independent of the flow times and durations, the maximum flow may be adjusted by placing a valve in the exit line.

Entry Applications

Application 1

Begin flow at time=0 with a step change and continue indefinitely.

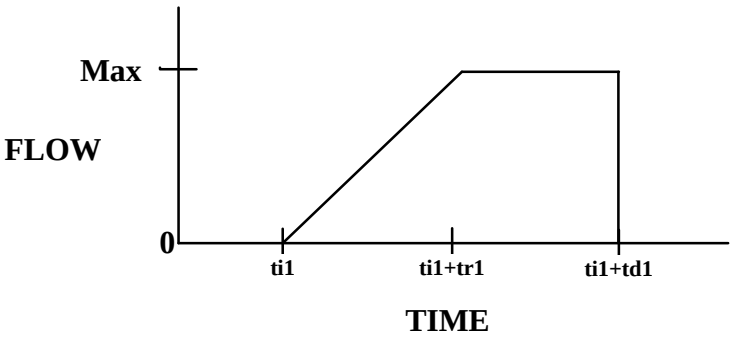


DynaChem Input: None Required

Requires no Input because all three entries (INITIATE, DURANON, and TRAMP are defaults.

Application 2

Begin flow at time=ti1 and reach maximum flow trl hours later (i.e., "ramp" time=tr1). Continue flow for tdl1 hours.



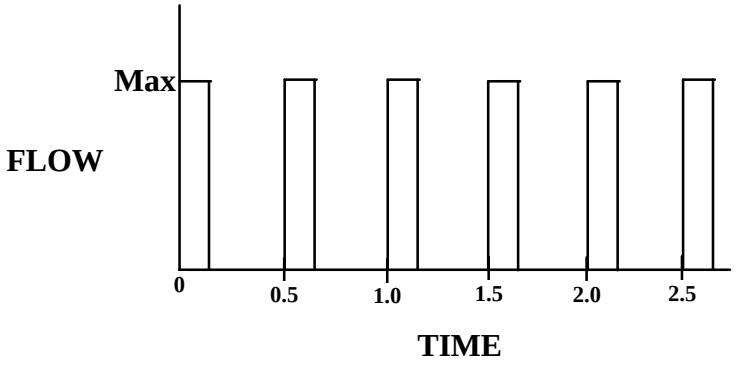
DynaChem Input: INITIATE=ti1

DURATION=td1

TRAMP=tr1

Application 3

Produce Intermittent 'slugs' of flow lasting 6 minutes (0.1 hour) each, occurring every 30 minutes (0.5 hour), the first occurring at time=0. All will be step changes.



DynaChem Input: INITIATE=0,0.5,1.0,2.0,2.5

DURATION=0.1,0.1,0.1,0.1,0.1

Since all are step changes (TRAMP=0,0,...) TRAMP may be omitted. The Input can be simplified, however, with the REPEAT Keyword as follows:

DynaChem Input: INITIATE=0

DURATION=0.l

REPEAT=0.5,1.0,1.5,2.0,2.5

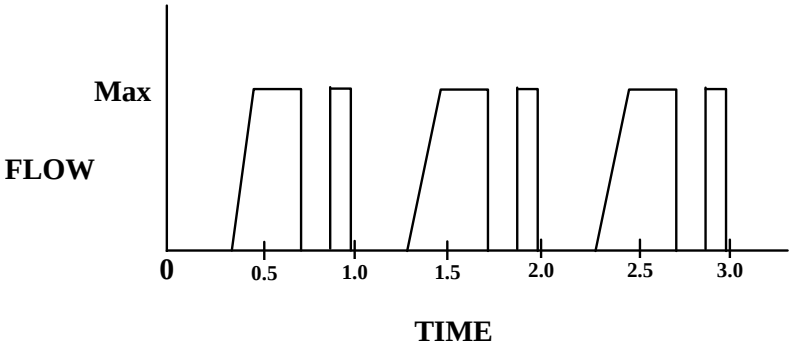
Furthermore, since all INITIATE entries are zero, the Keyword itself may be omitted:

DynaChem Input: DURATION=0. 1

REPEAT=0.5,1.0,1.5,2.0,2.5

Application 4

Begin a flow at time = 0.25 hour, reaching its maximum at time = 0.40 hour ("ramp" time 0.15 hour) and stop at time = 0.7 hour (duration = 0.45 hour). Start again at time = 0.85 hour, reaching maximum flow immediately (step change, ramp time = 0) and stop again at time = 0.95 hour (duration = 0.1 hour). This series of flows will repeat hourly.



DynaChem Input: INITIATE=0.25,0.85

DURATION=0.45,0.1

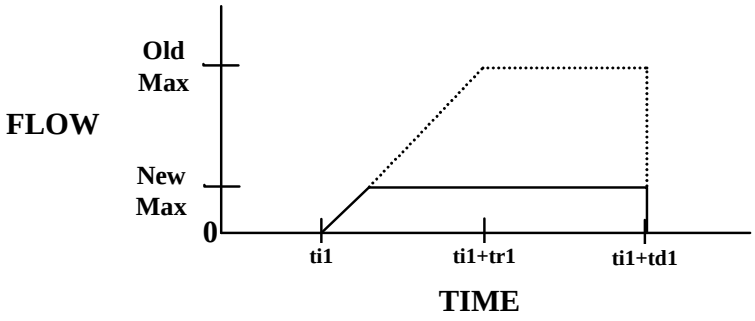
TRAMP=0.15

REPEAT=1,2,3,4

The REPEAT Keyword causes the INITIATE, DURANON, TRAMP series to be repeated starting at each of the specified times. Notice that the series begins at time = 0. Therefore, even though the flow does not begin until time = 0.25 hour, the specified Repeat times must coincide with time = 0. Thus, after the initial series, flow actually begins at time = 1.25 hour, 2.25 hour, etc.

Application 5

Suppose there is a valve in the exit line for the flow described in (2) above. Furthermore, suppose either the valve capacity (C_v) or the valve stem reduces the maximum flow to one-half of the maximum flow specified in the STATE specification.



The maximum flow is reduced to the maximum allowable by the valve. The rate at which the flow increases from zero to the STATE maximum does not change. That is, the slope of the Ramp does not change. Therefore, the effective ramp time, or the time at which the flow "levels off' is reduced.

Application 6

An ENTRY stream with a valve may be used for metering fluid from an "apparent" infinite supply. For example, the flow of Neutralization Reagent described in "Building a DynaChem Model" is from an Entry Unit. The maximum flow is set by the minimum of two values: (1) the STATE flow

and (2) the valve capacity (C_v). The flow is then regulated by adjusting the value stem as determined by the pH control loop.

Application 7

Scheduled flow is accomplished by using the flows as they occurred at a Node during a previous execution. For example, suppose you wished to analyze in two parts the Neutralization process described in "Building a DynaChem Model." The first part would end with Nodes 2 and 3 and the second part would begin with Node 2 (Node 3 is not an Upstream Node for any other Unit). The DynaChem Input for the first part would be as follows (refer to "Building a DynaChem Model" for the Input file as a single run):

```
SAVE      LOGNODE=2
TIME      TEND=1.0 TINC=0.0l
NODE      ORDER=1,2
PRINT     OUTPUT=10 SUMMARY=1
UNIT1     ENTRY DNODE=1 TRAMP=0.05 'PROCESS FEED'
          STAT'E = 25, 1, 40, 55.51, 0.01, 0.75, 0, 0.04
UNIT2     TANK UNODE=1 DNODE=2,3 LEXIT=0.25,3.5
          'SURGE TANK' CSA=7.07 MAXLEVEL=6
          STATE=20,1,20,1
VALV1     DNODE=2 CV=40
VALV2     DNODE=3 CV=50
CLOOI     VID=1 POSITIONAL SPUNIT=2 SPID=LEVEL
          SPVAL=1,3 KC=0.2 VCONSTANT=0.35
CLOO2     VID=2 SPUNIT=2 SPID=LEVEL SPVAL=4.5
          KC=0.5
```

The first line (SAVE LOGNODE=2) results in a Node Output file in which all state information describing Node 2 is saved for all time steps. At the conclusion of the execution, the Node Output file should be transferred to the Node Input file for the next execution. In most DynaChem versions, this may be done when exiting the Execution Procedure.

Once the Node Input file is acquired from execution of the first part (above), the second part may be executed with the following:

```
TIME      TEND=1.0 TINC=0.01
NODE      ORDER=2,6,5
PRINT     OUTPUT=10 SUMMARY=1
UNIT2     ENIRY DNODE=2 LOGNODE=2
```

```
UNIT3     TANK UNODE=2,5 DNODE=6 LEXIT=4
          'NEUTRALIZATION TANK'
          CSA=3.14 MAXLEVEL=4
          STATE=20,1,5.5,1
UNIT4     ENTRY DNODE=5 REAGENT FEED
          STAT'E = 20,1,5,.8988,0,0,.1012
VALV3     DNODE=5 CV=10
CLOO3     VID=3 SPUNIT=3 SPID=PH SPVAL=9
          KC= -0.01 TAUI=1
```

This second part must have all of the required Keywords (e.g., TIME), since only Node information has been stored. In the 4th line of this Input file, UNIT2 is an ENTRY with the temperature, pressure, total flow and composition specified by LOGNODE=2. The LOGNODE references the Node Number from the previous run (the Node Number that was stored). In the second part, UNIT2 has a DNODE=2, but the LOGNODE and DNODE need not be the same. Thus, as this second part is executed, the same mass and energy appears at Node 2 in this run as appeared at Node 2 in the first execution.

Since the first part was executed with TEND=1.0 TINC=0.01, values for Node 2 will be available for time = 0, 0.01, 0.02, 0.03,..., 1.0. The second part could be executed with different time parameters with the following restrictions:

1) Node values are available only to time=1.0. If the second part were run past that point, Node 2 would produce zero flow.

2) The time increment (TINC) for the second part must be less than or equal to the time increment for the first part.

Application 8

A rate-limited reaction is to occur in aqueous solution in a stirred reactor. However, one of the reactants (inflow species number 4) is to be metered into the reactor in its pure component form (i.e., non-aqueous). It is known that at the temperature and pressure of the Entry stream (25 °C and 1 atm), the fluid is liquid. The maximum flow will be 5 m^3/hr of the pure liquid. The DynaChem input for the Entry Unit should contain

STATE=25,1,5,0,0,0,1

NONSTANDARD=LIQ

All of the other Keywords apply the same as if the stream were aqueous and an equilibrium computation was to be made.

Furthermore, the stream may be multicomponent. The stream may contain any combination of the inflow species as long as each species which is specified in the STATE line does exist in the phase

designated. For example, if NaCl is specified in the STATE, then NONSTANDARD=SOL is acceptable. NONSTANDARD=VAP, however, would not be appropriate.

TANK UNIT

The TANK Unit may be used to represent any vessel or collection of mass and energy which may change in quantity and/or volume. Often this will be merely a tank, but the Tank Unit may also represent such diverse physical entities as the shell side of a boiler, a tray in a distillation column or a continuous stirred-tank reactor (CSTR).

The TANK is defined physically by (1) cross-sectional area, (2) maximum level, (3) maximum volume, (4) bottom volume, and (5) level of exits.

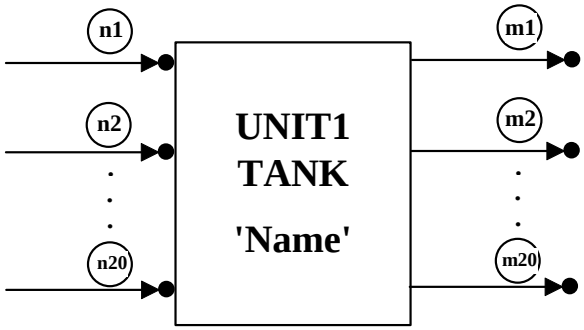
Assuming the tank is initially empty, the DynaChem Input for this Unit is as follows:

UNIT1 TANK UNODE=1 DNODE=3,2 LEXLT=2,10

CSA=7 MAXL=10

SUSP=0.0002 DISL=0.005 DISV=0.0005 ENTL=0.001

UNITi TANK



Specifications (Required):

UNODE=n1,n2,... Upstream Node Number(s) - maximum for Tank Unit is 20 (no minimum). May include Nodes entered as Energy Nodes (ENODE) in other Units.

DNODE=m1,m2.... Downstream Node Number(s) - minimum for Tank Unit is 1 and maximum is 10

STATE=T,P, Contents,xl, x2,... Defines initial state of fluid.
(Not required if tank is initially empty)
Order of entry:
Temperature (°C)
Pressure (atm)
Contents (m^3 or Alternate Units)
Alternate Contents Units: To enter alternate units, the numeric entry should be followed by (GRAM) for grams or (GMOL) for

	gmoles. Molar fraction, Inlet Comp 1 Molar fraction, Inlet Comp 2 . . . . . . Molar fraction, Inlet Comp N
CSA=v	Tank cross-sectional area (m2)
MAXLEVEL=v	Maximum tank level (m)
MAXVOL=v	Maximum tank volume (m^3)

Specification Note:

Any two of the three size specifications (CSA, MAXLEVEL, MAXVOL) are required. The third is computed by DynaChem.

Specifications (Optional):

LEXIT=vl,v2,...	Exit level of outlet line(s) from tank (m) in DNODE list order. (defaults)
BOTI'OM= v	Tank volume below tank zero level (m') (default = 0)
SUSPEND= v	Solids suspended in the liquid solution (gms solids/gms liquid) (default=infinite)
DISVAPOR= v	Vapor dissolved in the liquid solution (gms vapor/gms liquid)(default=0)
ENTLIQUID= v	Liquid entrained in the vapor (gms liquid/gms vapor) (default=0)
DISLIQUID= v	Liquid dissolved in the solid (gms liquid/gms solid) (default=0)
DISORGANIC= v	Organic liquid dissolved in aqueous liquid (gms organic liquid/gms aqueous liquid) (default=infinite)
DISAQUEOUS= v	Aqueous liquid dissolved in organic liquid (gms aqueous liquid/gms organic liquid) (default=0)
RXSTEPS= n	Number of Reaction (Kinetics) Steps overall time step (i.e., reaction time step = TINC/RXSTEPS) (default=1). To deactivate kinetics, set RXSTEPS=0.
RXTINC=tl,t2.,..	Reaction (Kinetics) time steps (hr). Up to four times may be specified. (Default=TINC/TXSTEPS). The sum of the RXSTEPS time steps must be TINC. Thus, a maximum of RXSTEPS-1 entries may be made. For less than RXSTEPS-1 entries, the remainder are equally divided.
NOVAP	Do not allow a vapor phase to be considered. (default = vapor allowed if present in Chemistry Model Definition)
NOEQ	Do Not Compute Equilibrium after time zero. Mass and energy is conserved, but temperature, pH, etc. are estimated. This may be used for tanks that have no inflows, such as reagent storage tanks. (default compute equilibrium at each time increment)
‘aaaaa’	Unit name

In computing the mass and energy at the downstream Nodes, first the mass and energy in the inflow streams are combined with the contents remaining in the tank from the previous time increment, the equilibrium condition is then computed.

From the equilibrium computation, the total volume of the combined mass is determined. From that volume, the tank level is determined. Mass and energy is placed at each downstream Node based

upon (1) exit level and (2) valve capacity and stem position. Vapor is separated from the fluid (liquid + solid) and is treated differently.

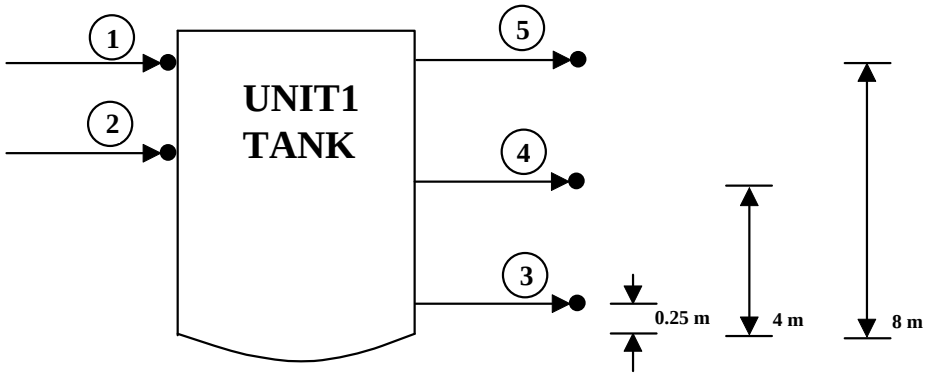
Fluid (liquid + solid) is placed at downstream Nodes from the lowest exit to the highest. Vapor is placed at downstream Nodes from the highest exit to the lowest.

A common use of the Tank Unit is a vessel in which several streams enter, are mixed with the existing contents and exit through multiple exits.

Application 1

Consider a tank with a diameter of 4 m and, therefore, a cross-sectional area of 12.57 m^2. The maximum level will be 8 m. The bottom of the tank will contain a spherical section with a volume of 3.2 m^3. That volume is below the zero level of the tank The maximum volume of the tank will be 103.7 m^3 (100.5 m^3 in the "straight-side" portion and 3.2 m^3 in the spherical section below).

There will be two feed streams (Nodes 1 and 2) and three exit streams (Nodes 3, 4 and 5, from bottom to top). The streams will exit at levels of 0.25 m, 4 m and 8 m, respectively.



Fluid (liquid + solid) may flow through an exit only if the fluid is at or above the level at which the exit is placed.

The lowest exit in this tank is at 0.25 m. Thus, for fluid to exit the tank the level must exceed

0.25 m which means the volume of fluid must exceed 6.3 m^3 (3.2 m^3 in the spherical section + 0.25 m * 12.57 m^2 in the straight-side section). Once the fluid exceeds that level, it will begin to flow through the exit. The amount of flow may be limited by two factors:

1. The volume of liquid which may flow during the time increment is the volume of fluid above the exit level.
2. The volume of fluid in any exit is limited by the valve capacity and stem position, if there is a valve. If there is no valve in the line, the flow is limited only by the available (i.e., fluid level).

Once the fluid level exceeds 4 m (the level of the second exit), the fluid may flow through both exits. The same two limitations (volume above the exit and valve capacity) apply to the higher exit as well.

When two or more exits "qualify" for fluid flow, fluid will flow preferentially from the lowest exit to highest exit. For example, if the level reaches 4.4 m, there is 5.0 m^3 of fluid above the 4 m exit and 52.2 m^3 of fluid above the 0.25 m exit. If there is no valve in either line, 52.2 m^3 of fluid will flow through the 0.25 m exit and no fluid will exit through. the 4 m exit. If there is a valve in the lower line, but 5.0 m^3 of fluid still exits through the lower line, then again, no fluid exits through the 4 m exit. If, however, due to a valve in the 0.25 m line, only 2 m^3 of fluid exits, then the remaining 3.0 m^3 may exit through the 4 m line (assuming that there is no valve or the valve has a large enough capacity).

The tank is described as Unit 1 with the following DynaChem Input:

UNIT1 TANK UNODE=1,2 DNODE=3,4,5 LEXIT=0.25,4,8

CSA=12.57 MAXLEVEL=8 BOTTOM=3.2

It should be noted that in the above discussion the term "flow" is often used. The actual quantity that is being described is the amount of mass being placed at a Node during the time increment. 'seat is, if the entire volume above an exit level "flows" through the exit, the reality is that the volume which is above that exit level, is "placed" at the Node. The volumetric "flow" is indeed, that volume divided by the time increment (TINC).

The above description of flow refers to "fluid". Fluid, in this case, includes the liquid and solid phases perfectly mixed. Vapor, however, is assumed to separate completely.

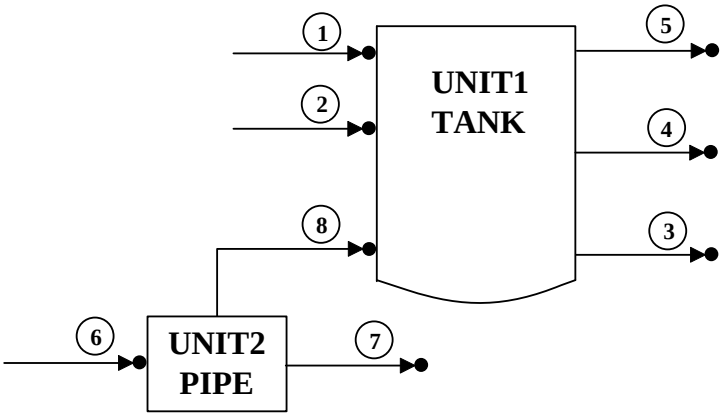
1) The vapor will exit preferentially from the top exit down to the bottom exit. In this case, the 8 m exit will receive vapor flow first, if any vapor exists.

2) The vapor will not exit through a line which is below the fluid (liquid + solid) level. In this case, if the fluid level is 4.4 m, the vapor may exit only through the top (8 m) exit.

3) In the same manner as fluids, the volume of vapor in any exit is limited by the valve capacity and stem position is there is a valve.

Application 2

All inlet and outlet streams in Application 1 have included both mass and energy. There are cases, however, when only energy is being transferred from one unit to another. For example, in the tank above, a cooling coil may be added. By including a Pipe Unit (UNIT2) with an inlet temperature of 20 °C (Node 6) and a discharge temperature (TDIS) of 40 °C (Node 7), the energy required to increase the temperature 20 °C will be "taken" (cooling) from the tank at Node 8. (Energy being "taken" at Node 8 is equivalent to Negative Energy being "added" at Node 8).



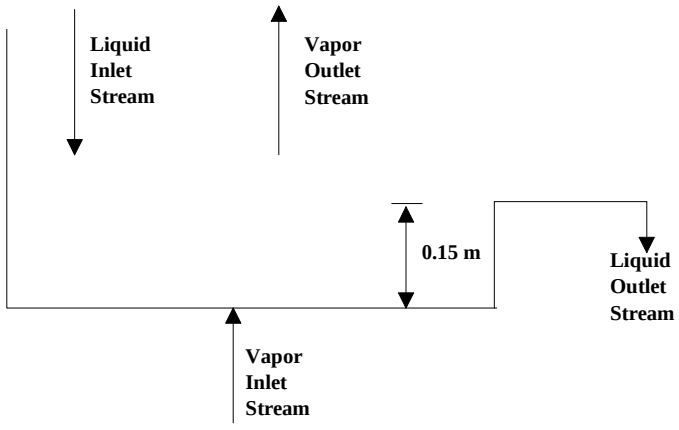
The above DynaChem Input becomes

```
UNIT1     TANK UNODE=1,2,8 DNODE=3,4,5 LEXIT=0.25,4,8
          CSA=12.57 MAXLEVEL=8 BOTTOM=3.2
UNIT2     PIPE UNODE=6 DNODE=7 ENODE=8 TDIS=40
```

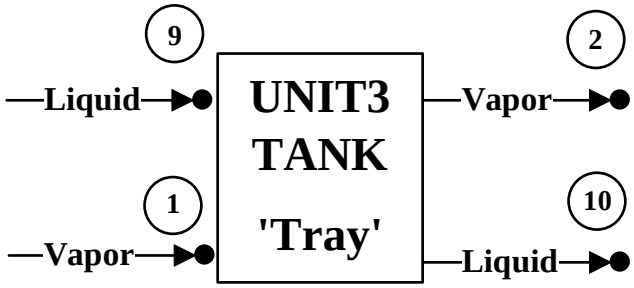
Node 8 is an Energy Node (ENODE). Energy Nodes are also discussed in the Pipe Unit Section.

Application 3

A distillation column tray may also be modeled with a Tank Unit. Consider a tray 1 m in diameter (cross-section area = 0.785 m^2) with an overflow baffle which is 0.15 m. Two streams (one liquid and one vapor) enter the tray and two streams (one liquid and one vapor) exit the tray.



The Liquid Outlet Stream (Node 10) will be placed at a level of 0.15 m with no valve. All fluid above that level will exit (i.e., overflow). The Vapor Outlet Stream (Node 2) may be placed at any level greater than or equal to 0.15 m to assure the departure of the vapor. Thus, once the tray fills, it will remain filled, just enough fluid leaving each time increment to maintain the fluid level at 0. 15 m. Meanwhile, all of the vapor evolved exits.



The tray is described as Unit 3 with the following DynaChem Input:

UNIT3 TANK UNODE=1,9 DNODE=10,2 LEXIT=0.15,.2

CSA=0.785 MAXLEVEL=.2

The maximum level has been set at 0.2 m. As long as the maximum level is above the overflow exit level, its only purpose is to assure a vapor exit since the level can never go above the overflow exit level of 0.15 m.

A distillation column may then be modeled by including several of these in series. In most cases, the inlet streams will be the outlet streams from the other Tank Units (trays).

Application 4

A tank is generating solids and vapor under conditions in which (1) a portion of the solids is suspended in solution and the remainder settles, and (2) the vapor velocity causes liquid to be entrained. In addition, liquid is dissolved in the settled solid, and vapor is dissolved in the liquid. All of these phenomena may be modeled with the Tank Unit.

The vapor, containing entrained liquid, will exit from the top of the tank (Node 2) at a level of 10 m. A lower exit (Node 3) will be located at 2 m. The liquid solution, containing suspended solids and dissolved vapor, will exit this line.

The default condition in both tanks and pipes is (1) 100% mixing of solids in the liquid solution (SUSP=infinite), (2) liquid entertainment (ENTL=0), (3) no liquid dissolved in the solid (DISL=0), and (4) no vapor dissolved in the liquid (DISV=0).

In this tank, after the equilibrium condition has been determined, the phases will be separated as follows:

1) All solids will settle to the bottom of the tank except 0.0002 gram of solid will be suspended in the liquid per gram of liquid (SUSP=0.0002).

2) In the settled solid, 0.005 gram of liquid will be dissolved per grain of solid (DISL=0.005).

3) All of the vapor will move to the top of the tank and exit the highest exit,. except 0.0005 grain of vapor will be dissolved per gram of liquid (DISV=0.0005).

4) The vapor exiting will contain 0.001 gram of entrained liquid per gram of vapor (ENTL=0.001).

5) After the liquid is dissolved in the solid and entrained in the vapor the remaining liquid (containing the suspended solids and dissolved vapor) may flow out the lower exit if the height of the fluid is 2 meters or greater.

Assuming the tank is initially empty, the DynaChem Input for this Unit is as follows:

```
UNIT1      TANK UNODE=1 DNODE=3,2 LEXLT=2,10
           CSA=7 MAXL=10
           SUSP=0.0002 DISL=0.005 DISV=0.0005 ENTL=0.001
```

Application 5

A CSTR is to be used in a process with other units. The rate-limited reaction (kinetics) in the reactor is a relatively fast reaction and requires a small time step (0.001 hour) to accurately model the reaction. The overall time constant for the process, however, is larger (0.01 hour) and TINC=0.001 would result in excessive computation time.

In this case, the time increment may be set at 0.01 hour and the reaction time step set at 0.001 hour with the following DynaChem Input:

```
TINC=      0.01
UNIT1      TANK UNODE=1 DNODE=2 CSA=5 MAXL=5
           STATE=25,1,10,1,.1
           RXSTEPS=   10
```

The reaction time step in the tank is computed as

Time Step = TINC / RXSTEPS

Since the default valve for RXSTEPS is 1, the default valve for the reaction time step would be TINC. In this case, the reaction time step will be 1/10 of TINC (0.001 hour).

Furthermore, since the unreacted inflows are added to the tank at the beginning of the time increment, the reaction rate is usually higher at the beginning of the overall time increment than at the end. Thus, it is typically more accurate to start with a lower reaction time step at the beginning of each time increment and decrease it through the increment. This is done with the RXTINC Keyword.

Set the reaction time steps as follows:

1st step: 0.00002 hour

2nd step: 0.0001 hour

3rd step: 0.0005 hour

4th through 10th steps: equally divided

The DynaChem partial Input will be:

```
TINC=     0.01
UNIT1     TANK UNODE=1 DNODE=2 CSA MAXL=5
          STATE=25,1,10,1,.l
          RXSTEPS=10 RXTINC=0.00002, 0.0001, 0.0005
```

By entering only the first three time steps, the 4th through 10th steps are assumed to be equal to TINC. The above will result in the total time increment for steps 4 through 10 being 0.00938 hour (0.01 - 0.00002 - 0.0001 - 0.0005), equally divided among the 7 reaction steps, results in a reaction time step of 0.00134 hour for steps 4 through 10.

PIPE UNIT

The PIPE UNIT is used to represent a process unit which maintains constant volume. This could be simply a section of pipe or it could be a tank heating/cooling coil, a shell-and-tube heat exchanger, a plug flow reactor or a filter.

The PIPE is defined physically by (1) cross-sectional area, (2) length, and (3) maximum volume.

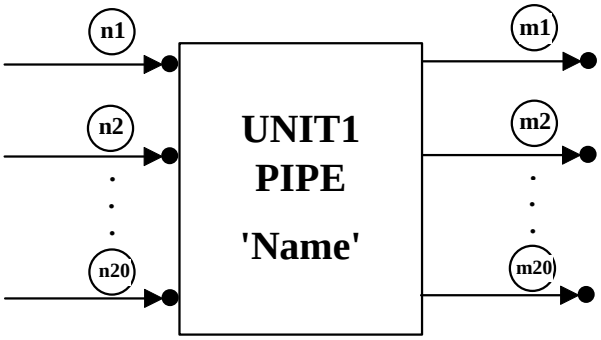
The total mass/energy at the downstream Node(s) is determined by the volume of material displaced by the inflows. The displaced mass/energy is at equilibrium and is homogeneous (i.e., all phases are mixed and flow as a single fluid). The state of the displaced material is identical to the state of the contents of the Pipe at the conclusion of the preceding time increment.

Downstream Nodes may be specified as liquid, vapor or solid allowing the displaced material to be separated by phase.

Warning: The Time Increment (TINC) must be small enough such that during no time increment shall Inflow volume be greater than the Maximum Pipe Volume (MAXVOL).

TINC< Maximum Pipe Volume/Peak Volumetric Flow

Schematic:



UNITi PIPE

Specifications (Required):

UNODE=nl,n2....	Upstream Node Number(s) - maximum for Pipe Unit is 20 (no minimum). May include Nodes entered as Energy Nodes (ENODE) in other Units.
DNODE=ml,m2,...	Downstream Node Number(s) - minimum for Pipe Unit is 1 and Maximum is 10. Should not include any Node entered as an Energy Node (ENODE) in this Unit.
STAT'E=T,P,Contents,xl,x2	Defines initial state of fluid. (Not Required if pipe is initially empty) Order of entry: Temperature (°C) Pressure (atm) Contents (m^3 or Alternate Units) Alternate Contents Units: To enter alternate units, the numeric entry should be followed by (GRAM) for grams or (GMOL) for gmoles. Molar fraction, Inlet Comp 1 Molar fraction, Inlet Comp 1 Molar fraction, Inlet Comp 2 . . . . Molar fraction, Inlet Comp N
CSA=v	Pipe cross-section area (m^2)
LENGTH=v	Pipe length (m)
MAXVOL=v	Maximum pipe volume (m^3)

Specification Note:

Either CSA and LENGTH must be entered or MAXVOL must be entered.

Specifications (Optional):

ENODE=n	An Energy Node which transports energy only (no Mass). When TDISCHARGE, TMAX or TMIN are used, any energy lost or gained can be transported to another Unit (the "Receiving Unit") via this "Energy Node." It should not be included as a DNODE for this Unit,, but should be included as a UNODE for the "Receiving Unit.'
TDISCHARGE=v	Discharge temperature (°C). Regardless of energy accumulated, the outlet temperature of the pipe is set to this temperature and the resulting energy is computed.
TMAX=v	Maximum temperature (°C). The outlet temperature is determined by an adiabatic flash. If the resulting temperature is less than TMAX, then it is used. If it is greater, the outlet is set at this temperature and the resulting energy is computed (e.g., a cooling exchanger).

TMIN=v	Minimum temperature (°C). The outlet temperature is determined by an adiabatic flash. If the resulting temperature is greater than TMIN, then it is used. If it is less, the outlet is set at this temperature and the resulting energy is computed (e.g., a heating exchanger).
LNODE=n	A liquid Node allows liquid (plus suspended solid and dissolved vapor) only.
SNODE=n	A Solid Node allows solid (plus dissolved liquid) only.
L2NODE=n	A 2nd Liquid Node allows organic liquid (plus dissolved aqueous, suspended solid, and dissolved vapor) only.

Specification Note:

When LNODE, VNODE and/or SNODE are specified, the total quantity of mass to be placed at the downstream Node(s) is determined first using the same phase proportions as exist in the Unit at the end of the previous time step. That total displaced quantity is then placed at the downstream Node(s) (in DNODE order) but with the LNODE, VNODE, SNODE restriction enforced on any designated Node. Furthermore, SUSPEND, DISVAPOR, ENTLIQUID and DISLIQUID may be used to modify what otherwise would be single-phase Nodes.

SUSPEND=v	Solids suspended in the liquid solution (gms solid/gms liquid) (default=infinite)
DISVAPOR=v	Vapor dissolved in the liquid solution (gms vapor/gms liquid) (default=0)
ENTLIQUID=v	Liquid entrained in the vapor (gms liquid/gms vapor) (default=0)
DISLIQUID=v	Liquid dissolved in the solid (gms liquid/gms solid) (default=0)
DISORGANIC=v	Organic liquid dissolved in aqueous liquid (gms organic liquid/gms aqueous liquid) (default=infinite)
DISAQUEOUS=v	Aqueous liquid dissolved in organic liquid (gms aqueous liquid/gms organic liquid) (default=0)
RXSTEPS=n	Number of Reaction (Kinetics) Steps per overall time step (i.e., reaction time step = TINC/RXSTEPS) (default=1). To deactivate kinetics, set RXSTEPS=0.
RXTINC=t1, t2,	Reaction (Kinetics) time steps (hr). Up to four time steps may be specified. (Default=TINC/RXSTEPS). The sum of the RXSTEPS time steps must be in TINC. Thus, a maximum of RXSTEPS-1 entries may be made. For less than RXSTEPS-1 entries, the remainder are equally divided.
NOVAP	Do not allow a vapor phase to be considered. (default = vapor allowed if present in Chemistry Model Definition)
NOEQ	Do Not Compute Equilibrium after time zero. Mass and energy is conserved, but temperature, pH, etc. are estimated. This may be used for pipes that are used only for process dead time. (default = compute equilibrium at each time increment)
‘aaaaa’	Unit name

The quantity of mass/energy at the downstream Node(s) is the amount of material which must be removed from the pipe such that when (1) the inflows are mixed with the material remaining, and (2) the equilibrium condition computed, then (3) the resulting volume is equivalent to the Maximum Pipe Volume. That is,

MPipe(t2) = FRAC * MPipe(t1) + MInflow(t2)

MNode(t2) = (1 - FRAC)*MPipe(t1)

MaxVol = Volume(MPipe(t2))

where:	t2	=t1 + One time increment
	MPipe(t2)	=Mass in Pipe at time t2
	MInflow(t2)	=Mass Inflow to Pipe during time increment t1 to t2
	MPipe(t1)	=Mass in Pipe at time t2 (i.e., contents of pipe at end of previous time increment)
	MNode(t2)	=Mass placed at Nodes during time increment t1 to t2
	FRAC	=Fraction of Pipe contents from previous time increment which remains in the Pipe
	MaxVol	=Maximum pipe volume
	Volume(MPipe(t2))	= Volume occupied by the Mass in Pipe at time t2
		=Specific Volume * Mass in Pipe

The known values in these equations are:

Mlnflow(t2) - defined by upstream Nodes

MPipe(t1) - computed in previous time increment

The unknown values in these equations are:

MPipe(t2) - Volume(Mpipe(t2)) is a direct function of the State of the Pipe contents

MNode(t2)

FRAC

The equations are solved simultaneously for the three unknowns. It should be noted that Inflows "force" material out of the Pipe. The inflows and previous contents ARE NOT MIXED before the material is forced out. This preserves the plug flow nature of the Pipe.

The following flow conditions can occur:

1) When the volume of the Inflows is less than the Maximum Pipe volume, FRAC is greater than 0 and less than or equal to 1.

1. When the combined Inflows (MInflow(t)) and previous pipe contents (MPipe(t1)) result in a volume GREATER THAN the Maximum Pipe Volume (MaxVol) then the value of FRAC is greater than 0 and LESS THAN 1. As FRAC increases from 0 to 1, the degree of Backmixing decreases and the mixing phenomenon proceeds from CSTR (FRAC=0) to Plug Flow (FRAC=1).

2. When the combined Inflows (MInflow(t2)) and previous pipe contents (Mpipe(t1)) result in a volume LESS THAN the Maximum Pipe Volume (MaxVol) then the value of FRAC in the above equation becomes GREATER THAN 1, which is physically impossible. In this case FRAC is set equal to 1 and, therefore, MNode(t2) = 0.

2) When the volume of the Inflows is exactly equal to the Maximum Pipe Volume, FRAC is equal to 0. In this case, no material is mixed (i.e., No Backmixing) and the extreme of pure Plug Flow is achieved.

3) When the volume of the Inflows is greater than Maximum Pipe Volume, FRAC is less than 0. This condition, of course, is illegal and an ALARM results.

The fluid in the pipe is totally mixed. If any vapor or solid phases exist at equilibrium, they will be mixed with the liquid phase. Consequently, since vapor has a significantly greater specific volume than the liquid and solid phases, the presence of vapor could have a significant impact on - the fluid leaving the pipe. In particular, the sudden occurrence of vapor could cause a "flash" effect in which a "slug" of fluid is forced out of the pipe.

Once the total displaced volume is determined, it is placed at the downstream Nodes in the following order:

1) For all downstream Nodes with a valve, the allowable volumetric flow through the valve is computed and that volume of mixed fluid is placed at the Node. If the Node is designated with LNODE, VNODE or SNODE, only the appropriate phase (with modifications by SUSPEND, etc.) is placed at the Node. This procedure proceeds through the DNODE list (in order) for all exits with valves until the entire displaced volume has been distributed.

2) If any displaced volume remains after -all downstream Nodes with valves have been computed, all of the remaining flow is placed at the first downstream Node (in the DNODE list) without a valve. If that Node is designated with LNODE, VNODE or SNODE, then the appropriate phase is placed at the Node and the remaining flow is placed at the next downstream Node without a valve.

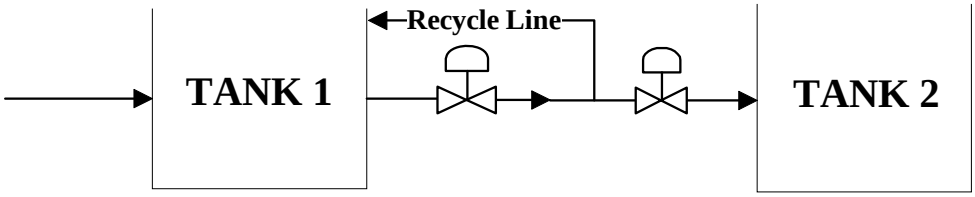
Care should be taken to provide sufficient capacity in the exit lines. Since the total volume leaving the pipe is a function of the volume displaced by the inflows (as compared to the TANK in which the volume leaving the tank is a function of the exit lines), if all downstream Nodes have valves, it is possible to exceed the capacity of the exit lines. Therefore, either one exit should remain without a valve or one valve should have a very large capacity.

Application 1

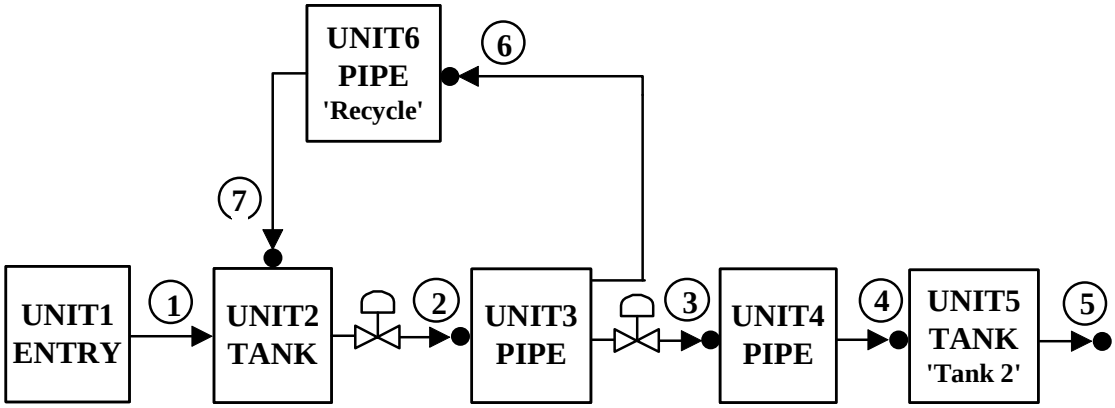
The simplest use of the Pipe Unit is as a section of pipe. This application results in process dead time and reduces backmixing. A series of pipes will (1) delay the impact of a "wave front" (e.g.,

temperature, pH, composition) one time increment for each Pipe Unit employed, and (2) increase the amplitude of the "wave front", compared to one large pipe or a tank, by reducing the dilution effect.

As an example, consider a tank with a recycle line.



To accurately represent the dead time in the recycle line and the line connecting the tanks, the following DynaChem model may be used:



VALV1 represents the valve on the exit line from Tank 1. Unit 3 includes the pipe volume from the exit of Tank 1 to the point at which the recycle lines splits (0.5 m^3). Unit 4 is the pipe volume between the split and Tank 2 (0.75 m^3). Unit 6 is the recycle line volume (1.5 m^3). Each of these sections will initially be filled with water at 20°C. The tanks are initially empty.

```
UNIT1    ENTRY DNODE=1 STATE=80,1,5,1.0,0.2,0.001,0.05
UNIT2    TANK UNODE=1,7 DNODE=2 'TANK 1' CSA=28
         MAXLEVEL=8
UNIT3    PIPE UNODE=2 DNODE=3,6 MAXVOL=0.5
         STATE=20,1,0.5,1
UNIT4    PIPE UNODE=3 DNODE=4 MAXVOL=0.75
         STATE=20,1,0.75,1
UNIT5    TANK UNODE=4 DNODE=5 'TANK 2' CSA=78
         MAXLEVEL=10
UNIT6    PIPE UNODE=6 DNODE=7 MAXVOL=l.5 'RECYCLE'
         STATE=20,1,1.5,1
```

VALV1 DNODE=2 CV=50

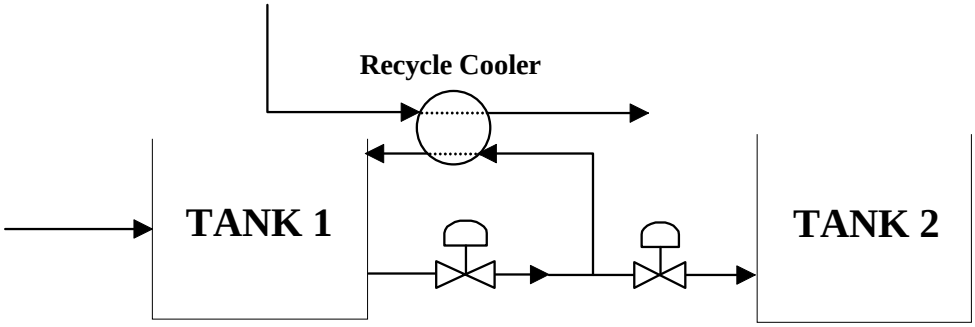
VALV2 DNODE=3 CV=20

NODE ORDER=1,2,3,4,5,7

Note that Node 6 does not need to be included in the Node Order since inclusion of Node 3 will result in Unit 3 and all of its downstream Nodes being computed.

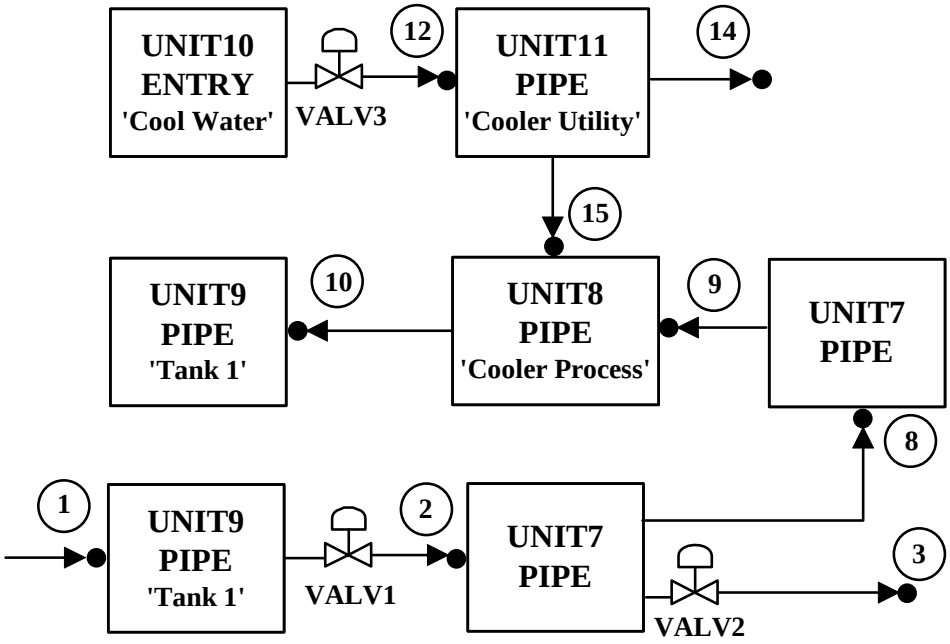
Application 2

An important attribute of the Pipe Unit is the combination of temperature specification (TDISCHARGE, TMAX and TMIN) and the Energy Node (ENODE). Suppose the Recycle line in Application 1 contains an inline cooler.



The cooler will be a shell-and-tube exchanger with a holdup of 0.7 m^3 on the process (recycle) side. Also, there will be 0.4 m^3 of pipe volume on each end of the cooler. The cooling water side will consist of 10 m^3/hr of pure water at 10°C. It will be assumed that sufficient heat transfer occurs to result in a cooling water temperature increase of 15°C (TDISCHARGE=25). Unless the specified discharge temperature is indeed the adiabatic equilibrium temperature (which it is not in this case), there will be a net gain or loss of energy by the Unit. If an Energy Node (ENODE) is included with the Unit, that energy flow caused by the temperature change is placed at that Node. No mass is placed at the Energy Node.

In this case the energy will be transferred from Unit 11 with Node 15 (ENODE=15). The Receiving Unit for the energy transfer will be Unit 8 (UNODE=15). The energy transferred from Unit 11 to Unit 8 will be "negative" energy in that the flow of energy will actually be from Unit 8 to Unit 11. That is, the enthalpy of the contents of Unit 11 will increase and the enthalpy of the contents of Unit 8 will decrease.




```
UNIT1     ENTRY DNODE=1 STATE=80,1,5,1.0,0.2,0.001,0.05
UNIT2     TANK UNODE=l,ll DNODE=2 'TANK l' CSA=28
          MAXLEVEL=8
UNIT3     PIPE UNODE=2 DNODE=3,8 MAXVOL=0.5 STATE=20,1,0.5,1
UNIT7     PIPE UNODE=8 DNODE=9 MAXVOL=0.4 STATE=20,1,0.4,1
UNIT8     PIPE 'COOLER-PROCESS'
          UNODE=9,15 DNODE=10 MAXVOL=0.7
          STATE=20,1,0.7,1
UNIT9     PIPE UNODE=10 DNODE=11 MAXVOL=0.4
          STATE=20,1,0.4,1
UNIT10    ENTRY 'COOL WATER'
          DNODE=12 STATE=10,1,10,1
UNIT11    PIPE 'COOLER-UTILITY' TDISCHARGE=25
          UNODE=12 DNODE=14 ENODE=15 MAXVOL=0.75
          STATE=10,1,0.75,1
```

VALV1 DNODE=2 CV=50

VALV2 DNODE=3 CV=20

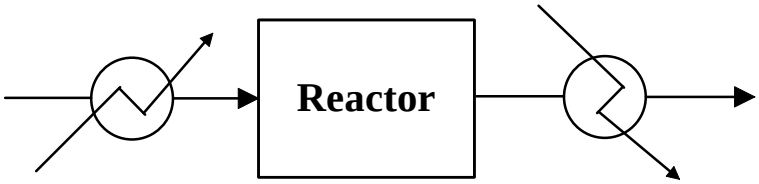
VALV3 DNODE=12 CV=10

NODE ORDER=1,2,8,9,12,14,10,11

If desired, a temperature control loop may be used to measure the discharge temperature of the process stream (Node 10) and adjust the cooling water flow with the valve (VALV3) on the exit of Unit 10 (Node 12).

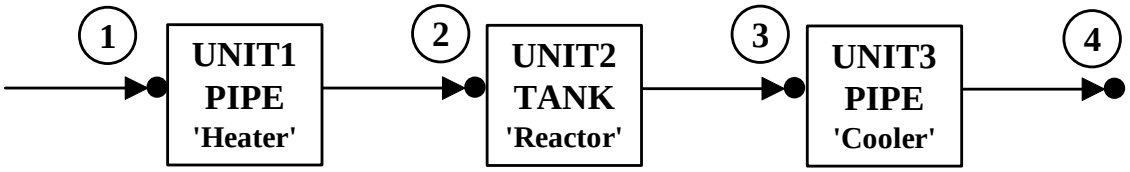
Application 3

Suppose a Reactor requires a heater on the inlet and a cooler on the outlet.



You may not, however, be interested in the utility side of the exchangers. You assume that the utilities and exchangers will be adequate to achieve the specified temperatures.

In this case the Reactor inlet temperature must be 30°C or greater (TMIN=30) and the fluid leaving the process must be 60°C or less (TMAX=60).



UNIT1 PIPE UNODE =1 DNODE=2 ‘HEATER’ TMIN=30

MAXVOL=0.5

UNIT2 TANK UNODE=2 DNODE=3 ‘REACTOR’

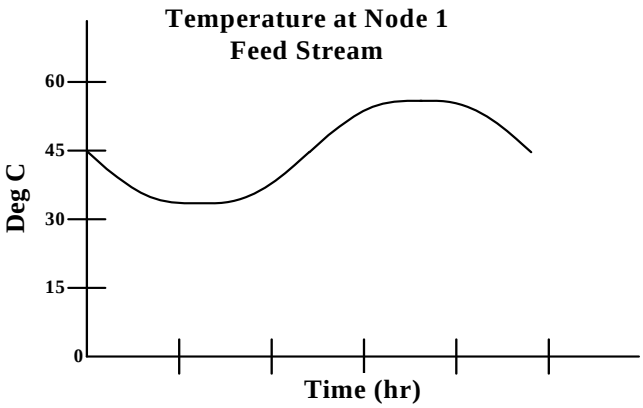
CSA=78 MAXLEVEL=10

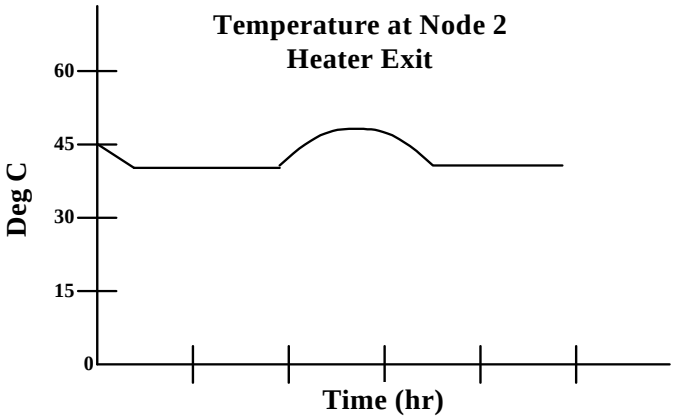
UNIT3 PIPE UNODE=3 DNODE=4 'COOLER' TMAX=60

MAXVOL=0.5

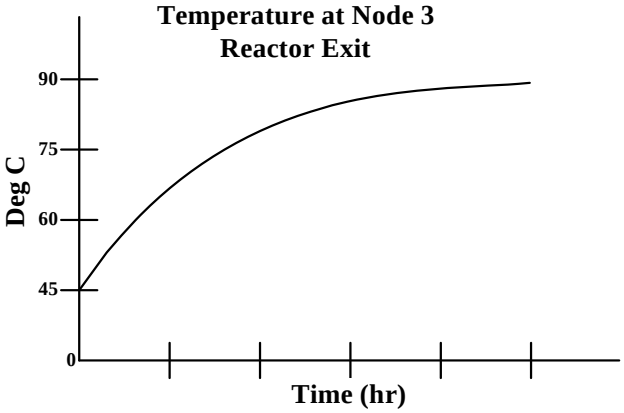
NODE ORDER=1,2,3,4

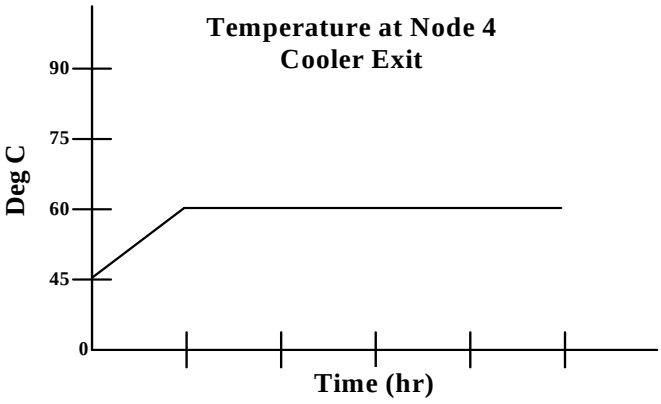
Suppose the temperature at Node 1 (Feed Stream) varies from 15°C to 50°C as shown in the first plot. The resulting temperature at the Heater exit (Node 2) is as shown in the second plot.





As the exothermic reaction proceeds, the Reactor temperature increases and the exit temperature (Node 3) increases from 35°C to 90°C. This increase is shown in the first plot below. The Cooler exit (Node 4) is maintained at a maximum of 60°C shown in the second plot.



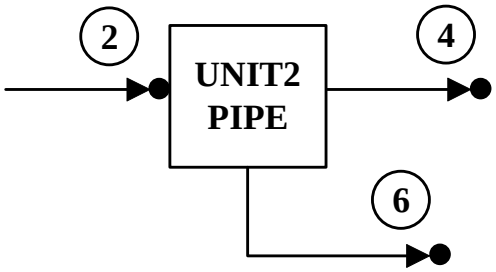


Application 4

By partitioning a tubular reactor into sections, each one represented by a Pipe Unit, plug flow characteristics (reactor backmixing) can be accurately modeled.

Coupled with ProChem's Reaction Kinetics capability, DynaChem can be used in this manner to model a complex Plug Flow Reactor.

Application 5



A filter is to be modeled in which the liquid leaving the unit is to be placed at Node 4 and the solid leaving the unit is to be placed at Node 6.

There will, however, be some solid suspended in the liquid (0.005 gram of solid per grain of liquid) and some liquid dissolved in the solid (0.001 gram of liquid per gram of solid).

The filter may be described by the following DynaChem input:

```
UNIT2 PIPE UNODE=2 DNODE=4,5 LNODE=4 SNODE=6
      STATE=50,1,14,1 CSA=0.5  MAXV=14
      SUSP=0.005 DISL=0.001
```

Note that although LNODE and SNODE are used for Nodes 4 and 5, they still must be included in the DNODE list.

Chapter 4: VALVE SPECIFICATION

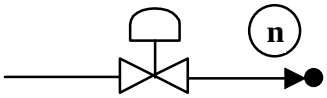
A VALVE is used to restrict the flow of mass and energy and, therefore, the amount of mass and energy which may be placed at a Node during a time increment. A Valve may be used preceding any Node, but only one Valve may be used before any Node.

The Primary Keyword (in abbreviated form) is

VALVi

where i represents a unique identification number from 1 to 50.

Schematic:



Each Valve must be associated with a downstream Node and a maximum capacity must be specified:

VALVi `DNODE=n CV=v

Specifications (Required):

DNODE=n	Downstream Node Number-minimum and maximum number of DNODE's for a Valve is 1.
CV=v	Valve capacity (m^3/hr)

Specifications (Optional) :

VOPEN=v	Valve override (Stem position until changed by Control Loop intervention) (default = 0, closed)
LINEAR	Linear valve (default = Linear)
EQUAL	Equal percentage valve (default = Linear)
RANGEABILITY=v	Rangeability (1/Rangeability = valve opening with fully closed stem position) (default = Infinitely large when Linear; Required when Equal percentage)
HYSTERESIS=v	Hysteresis Deadband (Fraction of Stem Movement) (default=0)
STICK=v	Valve Stick/Slip (Fraction of Stem Movement) (default=0)

PFCN=v Pressure function (default = 0)
= 0 f(p) = 1.0
= 1 f(p) = (Pu-Pd)**.5
= 2 f(p) = (Pavg(Pu-Pd))**.5

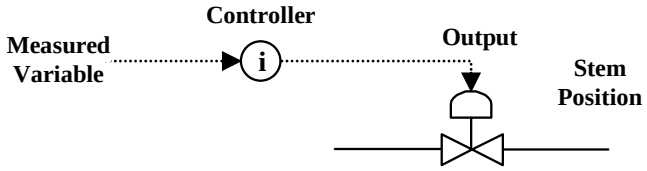
Chapter 5: CONTROL LOOP SPECIFICATION

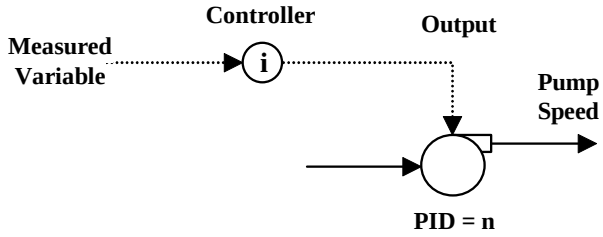
In general, a Control Loop (1) measures a process variable (temperature, pressure, pH, level, flow or composition) from a specified Unit or Node, (2) compares that value to a specified Setpoint and, as a result, (3) makes adjustments to a Valve (Stem Position), a Pump (Speed) or another Control Loop (Setpoint). Control Loops may also acquire information form another Control Loop rather than a Unit or Node.

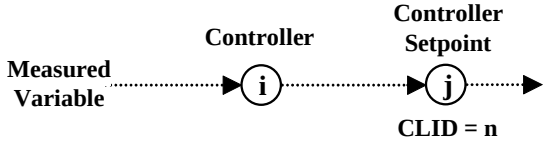
Various controller algorithms are available including (1) Velocity, (2) Positional (including Deadband), (3) Switch, (4) Multicascade, (5) Ratio and (6) Trim.' Each of these algorithms is described in one of the following sections.

For PID controllers, the Gain, Integral time and Derivative time are selected by the User but may be changed during execution for "tuning" purposes. Dead Time, Controller Output Limits and Controller Output Factors may be specified. Each of these is described in detail in the Algorithm Section in which it applies.

Schematic:







The Primary Keyword (in abbreviated form) is

CLOOi

where i represents a unique identification number from 1 to 50.

The maximum flow is set by the Valve Capacity and the actual flow is determined by the Valve Stem Position (fraction open). The Stem Position may be set by the User (manual) or by a Control Loop (automatic).

The valve override (VOPEN) should be used to set the initial Stem Position whether the Valve is to be manual or automatic. If, however, the Valve is initially closed it is unnecessary since the default is closed. VOPEN can also be used to change the Stem Position at specified times during an execution using (TIME=v) specification. For example, suppose Valve 1 is to be 10% open initially; but after 0.25 hour the stem Position is to be changed to 50% open:

VALV1 DNODE=1 VOPEN=0.l VOPEN=0.5 (TIME=0.25)

The (TIME=0) following VOPEN=0.l is omitted because it is the default.

The flow through a Valve is computed as follows:

Flow = Port * C_v * Pfac

where: Flow = Flow through valve, m^3/hr

Port = Valve port opening, fraction open

C_v = Valve capacity, m^3/hr

Pfac = Pressure factor, dimensionless

1) The Valve may be specified as a Linear Valve (default) or an Equal Percentage Valve. The type of Valve and the Rangeability (R) are used to convert the Valve Stem Position (Stem) to the Valve Port Opening (Port):

   Linear Valve: Port = (1/R) + [1-(1/R)]

   Equal Percentage Valve: Port = R ** (Stem - 1)

2) The Valve Pressure Factor (Pfac) is determined based upon the Pressure Function (PFCN) specified by the User:

   For PFCN = 1: Pfac = 1.0

   For PFCN = 2: Pfac = (Pup - Pdown)**.5

   For PFCN = 3: Pfac = (Pavg * (Pup - Pdown))**.5

   where:

   Pup = Upstream pressure (atm)

   Pdown = Downstream pressure (atm)

Pavg = Average pressure (atm)

Typically PFCN=2 is used for liquid streams and PFCN=3 is used for gas and vapor.

Specifications (Required):

VID=n	Valve ID to which Control Loop output is to be sent
CLID=j	Control Loop ID to which Control Loop output is to be sent
PID=m	Pump ID to which Control Loop output is to be sent

Specification Note:

The output of each Control Loop must have a destination. Thus, each Control Loop must have either a VID, CLID or PID. In some cases, the Control Loop may have two destinations (e.g., when the output is to be sent to a Valve and to a Multicascade Controller, both VID and CLID would be used).

Specifications (Optional):

VELOCITY	Velocity algorithm - PID Control (Controller Output = Stem Movement Distance)
POSITIONAL	Positional algorithm - PID Control (includes Deadband) (Controller Output = Stem Position)
SWITCH	Switch algorithm (Controller Output = Stem fully open or fully closed)
MULTICASCADE	Multicascade algorithm (Controller Output = sum of up to 5 Stem movements determined by other Control Loops)
RATIO=V	Ratio Control algorithm with a ratio value of v (Controller Output = Ratio * measured Value)
TRIM=vl,v2	Trim Controller algorithm with limits of v1 to v2. (Controller Output = 1 when the referenced valve stem position is within limits. Controller Output > 1 or < 1 when referenced valve stem position is outside limits.)

Specification Notes:

Each of the above Specification Keywords designates a different control algorithm. Only one algorithm may be specified for each Control Loop. The default algorithm is Velocity.

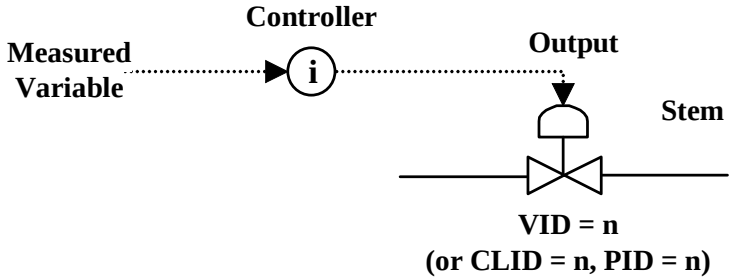
Each algorithm is described in detail in an individual section. The Specification Keywords required for each of algorithms are also described in those sections. Reference Table 4 provides a summary of Required and Optional Specification Keywords for each algorithm.

VELOCITY ALGORTHM

The Velocity algorithm is a PID Controller producing an output in Stem Movement distance.

Since the Output is a derivative-type function (ΔStem), a Valve Constant (Bias) is not required and Windup does not occur. Both of these are factors in the Positional algorithm.

Setpoint Specification is required and PID parameters are necessary. Dead Time and Output Limits are optional.



Schematic:

CLOOi VELOCITY

where i represents a unique identification number from 1 to 100.

Specifications (Required):

VELOCITY	Velocity algorithm - PID Control (Controller Output = Stem Movement distance)
VID=n	Valve ID to which Control Loop output is to be sent
CLID=n	Control Loop ID to which Control Loop output is to be sent
PID=n	Pump ID to which Control Loop output is to be sent
SPUNIT=n	Setpoint Unit ID (used with SPID=TENT, PRES, pH, LEVEL or COMP)
SPNODE=n	Setpoint Node ID (used with SPID=TEMP, PRES, pH, FLOW or COMP)
SPID=a	Setpoint Value ID SPID = TEMP for Temperature (°C) SPID = PRES for Pressure (atm) SPID = pH for pH SPID = LEVEL for Level (m) (may not be used with SPNODE) SPID = FLOW for Flow (m^3/Hr) (may not be used with SPUNIT) SPID = COMP for Composition (SPCOMP also required)
SPVAL	Setpoint value (default = 0)
KC=v	Gain (default = 0) - See Also: TAUI and TAUD (Gain > 0 for Direct Action; Gain < 0 for Reverse Action - See Algorithm definition below)

Specification Notes:

Since VELOCITY is the default algorithm, it is not necessary for it to appear as a Specification.

The output of each Control Loop must have a destination. Thus, each Control Loop must have either a VID, CLID or PID. In some cases, the Control Loop may have two destinations (e.g., when the output is to be sent to a Valve and to a Multicascade Controller, both VID and CLID would be used).

Inputs (i.e., Measured Values) of Control Loops must have a source. Thus, each Control Loop with Velocity algorithm must have a SPID and either a SPUNIT of SPNODE.

Specifications (Optional):

SPCOMP= Name, Units, Phase Setpoint Composition Specifications
(Required when SPID=COMP)
Name= Species, Inflow or Base Name (When Species is used, must be AQ or ION and Phase must be Liquid; when Base Name is used, such as CO2, refers to same as inflow such as CO2IN)
Units = Composition units
= WTFR for weight fraction
= MOLF for mole fraction
= MOLA for molality (species only)
= GMOL for gmoles
= GRAM for grains
Phase = Composition phase (when Name=Species, Liquid only)
= TOT for total (all phases combined) (not available with Species)
= LIQ for liquid
= VAP for vapor (not available with Species)
= SOL for solid (not available with Species)

TAUI=v Integral time (min) (default = 0)

TAUD=v Derivative time (min) (default = 0)

DEADTIME=v Dead Time from process measurement to Output or Stem action (hr) (default = 0)

KCPOLY=A,B,C,D Variable Gain coefficients - Polynomial form (default=0 for all coefficients)
Kc = A + B*MV + C*MV**2 + D/MV
MV = Value of Measured Process Variable

KCEXP=A,B,C,D Variable Gain coefficients - Exponential form (default=0 for all coefficients)
Kc = A + B / (C + exp(-D*MV))
MV = Value of Measured Process Variable

OLIMIT=v1,v2 Controller Output limits - low limit (v1) and high limit (v2). (default=No limits, except Stem may not result in stem position < 0 or > 1)

CFACTOR=V Controller Output Factor. When Output is to be sent to another Controller as specified in CLID, the Input to that Controller is the Output from this Controller multiplied times the Controller Output Factor. (default=l)

Specification Note:

The most common use of CFACTOR is when the output of the Control Loop is to be the input to a Multicascade Controller. In that case, the output from this Control Loop may be weighted at some value between 0 and 1, along with the output from other Control Loops providing input to the Multicascade Controller.

Velocity Algorithm Definition

Stem Movement at time j= ΔStem

= Stem Fraction Open at time j- Stem Fraction Open at time j-1

Note: Stem may not result in a Stem Position less than 0 or greater than 1.

$$Stem = Kc\left[\begin{array}{l}\left(ERROR(j) - ERROR(j-1)\right) \\ + \dfrac{TauD}{60} * \left(\dfrac{(ERROR(j) - ERROR(j-1)}{TIME(j) - TIME(j-1)} - \dfrac{ERROR(j-1) - ERROR(j-2)}{TIME(j-1) - TIME(j-2)} \right) \\ + \dfrac{60}{TauI} * ERROR(j) * (TIME(j) - TIME(j-1))\end{array}\right]$$

where ERROR(j) = Measured Value - Setpoint Value at time j

= Gain

= Change in Stem Position / Unit Error

When Gain > 0 Direct Action Control

When ERROR is Positive, Stem => 1.0, Open Valve. For example, Level Control.

When Gain < 0 Reverse Action Control

When ERROR is Positive, Step => 0.0, Closed Valve. For Example, pH Control of acid waste with NaOH - as pH increases above Setpoint, ERROR is positive and Valve closes.

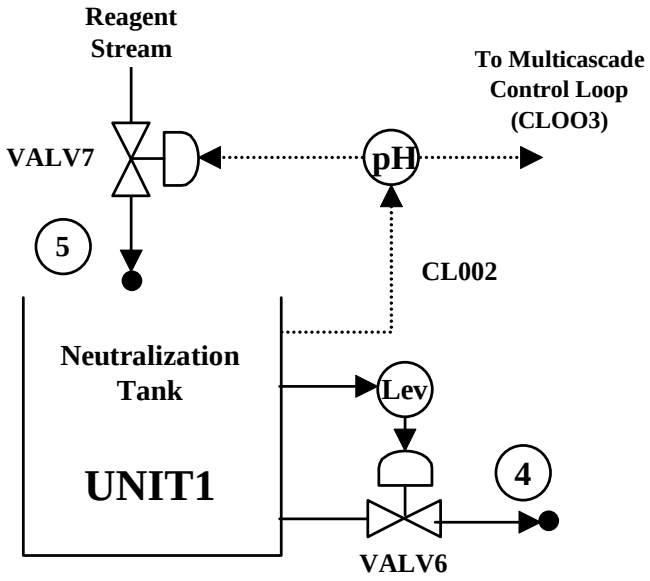
TauI = Integral time (min)

TauD = Derivative time (min)

Application 1

Two common applications of the Velocity algorithm are level control and pH control. Consider a Neutralization Tank with the need to maintain level and pH closely to specific setpoints.

In this case, level is controlled by (1) measuring the level in the Neutralization Tank (UNIT1), (2) the Control Loop (CLOO1) compares it to the Setpoint and (3) sends a Stem Position change to the valve (VALV6). Similarly, pH is controlled by (1) measuring the pH in the Neutralization Tank (UNIT1), (2) the Control Loop (CLOO2) compares it to the Setpoint and (3) sends a Stem Position change to the valve (VALV7). The output from the pH Control Loop (CLOO2) will also be sent to a Multicascade Control Loop (CLOO3).



The Tank level Setpoint (SPVAL) will be set at 3 m. The Error is defined as:

Error = Measured Level - Setpoint

The controller Gain (KC) will be 0.15. For a Velocity controller with Proportional only (i.e., Kc only, without TauI, or TauD):

Stem Position Change = Kc * (Error(j) - Error(j-1))

where Error(j) is the Error for the current time increment and Error(j-1) is the Error for the previous time increment

Thus, the Stem will open an additional 0.15 (i.e., 15%) for every additional movement of I m of level (1 Error unit) above Setpoint and will close 0.15 for every additional movement of I m below the setpoint. In this case, the units of Kc are:

Fractional Change of Stem Position/Level Change in Meters

Kc is possible since the Control Loop is to be Direct Acting. That is, as the Error increases (level moves above Setpoint), the Valve Stem Position must increase (increase tank exit flow).

In the pH Control Loop, the Setpoint will be 9. The controller Gain will be -0.1. In this case, the Gain is negative since the Control Loop is to be Reverse Acting. That is, as the Error increases (pH moves above Setpoint), the Valve Stem Position must decrease (reduce NaOH flow).

The level Control Loop will also have an Integral time of 2 minutes and the pH Control Loop will have an Integral time of 1 minute. Since the Velocity algorithm is a derivative-type function, the Integral action becomes a reflection of the most recent Error (see Velocity Algorithm Definition above).

Because of the mixing characteristics of the tank, Dead Time of 0.025 hour will be included in the pH Control Loop. In addition, both of these loops will have implicit Dead Time implications (See Dead Time).

CLOO1 VID=6 SPUNIT=1 SPID=LEVIEL SPVAL=3
KC=0.15 TAUI=2

CLOO2 VID=7 CLID=3 SPUNIT=L SPID=PH SPVAL=9
KC= -0.l TAUI=1 DEAD TIME=-0.025

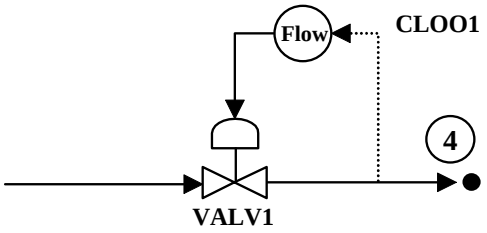
VALV6 DNODE=4 CV=30

VALV7 DNODE=5 CV=20

It is important to remember that the Control Loop sets the Valve Stem Position, which ranges from 0 to 1. The Valve Stem Position is then converted to the Valve Port Opening (See VALVE SPECIFICATIONS), which also ranges from 0 to 1. The Port is then applied, along with the Valve Pressure Factor, to the Valve Capacity (C_v) to determine the actual flow. The Valve Capacity not only sets the maximum flow, but for a given Stem Position change, its magnitude sets the rate of change of the flow.

Application 2

Although the Positional algorithm is often used for flow control, the Velocity algorithm is effective in many cases. In this case, the flow at Node 4 will be controlled with a valve (VALV1) immediately preceding it.



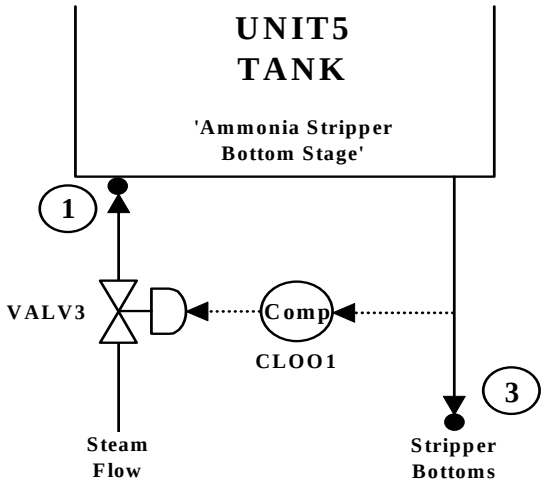
The Setpoint will be 5 m^3/hr. The Gain (KC) will be -0.075 (Reverse Acting).

CLOO1 VID=1 SPNODE=4 SPID=FLOW SPVAL=5
KC=-0.075

VALV1 DNODE=4 CV=10

Application 3

NH3 in the bottoms stream of an Ammonia Stripper is to be controlled by adjusting the steam rate to the stripper with an inlet valve (VALV3).



The bottoms stream is equivalent in composition to the liquid on the bottom stage (UNIT5). The measured variable (COMP) will be the mole fraction (MOLF) of NH3 in the liquid phase (LIQ). The Setpoint for the NH3 mole fraction will be 0.002 (0.2 mole %).

As the NH3 mole fraction increases, the steam rate must increase. Therefore, the Controller will be Direct Acting. A Gain of 400 will be used. Since the Gain is defined as

Kc = Fractional Change of Stem Position/Error

In this case, a fractional change in the Stem Position of 0.1 (10%) corresponds to a change of 0.00025 in the NH3 mole fraction. (i.e., 400 = 0.1 / .00025).

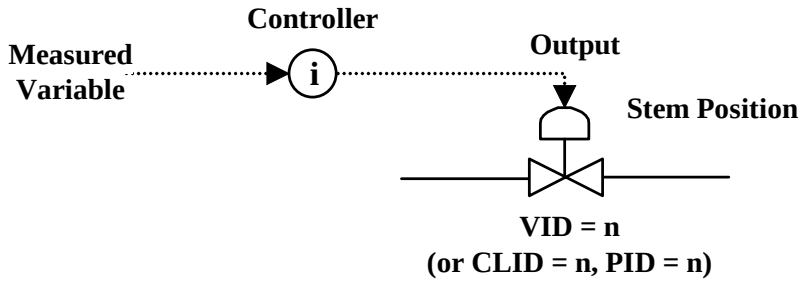
An Integral time (TAUI) of 0.5 minute is also included.

```
CLOO1     VID=3 SPUNIT=5 SPID=COMP
          SPCOMP=NH3,MOLF,LIQ SPVAL=0.002
          KC=400 TAUI=0.5
VALV3     DNODE=1 CV=1000
```

POSITIONAL Algorithm

The Positional algorithm is a PID Controller producing an Output in absolute Stem Position (Fraction Open). This Algorithm may also be used for Deadband Control.

Setpoint Specification is required and PID parameters are necessary. A Valve Constant (Bias) is required and Windup can occur is Integral time (TAUI) is used unless NOWINDUP is specified. Dead Time and Output Limits are optional.



CLOOi POSITIONAL

where i represents a unique identification number from 1 to 100.

Specifications (Required):

POSITIONAL	Positional algorithm - PID Control (includes Deadband) (Controller Output = Stem Position)
VID= n	Valve ID to which Control Loop output is to be sent
CLID= n	Control Loop ID to which Control Loop output is to be sent
PID= n	Pump ID to which Control Loop output is to be sent
SPUNIT= n	Setpoint Unit ID (used with SPID=TEMP, PRES, PH, LEVEL or COMP)
SPNODE= n	Setpoint Node ID (used with SPID=TEMP, PRES, PH, FLOW or COMP)
SPID=a	Setpoint Value ID SPID = TEMP for Temperature (°C) SPID = PRES for Pressure (atm) SPID = PH for pH SPID = LEVEL for Level (m) (may not be used with SPNODE) SPID = FLOW for Flow (m^3/Hr) (may not be used with SPUNIT) SPID = COMP for Composition (SPCOMP also required)
SPVAL=vl,v2	Setpoint value(s) (defaults=0,0)
KC=v	Gain (default = 0) - See Also: TAUI, TAUD (Gain > 0 for Direct Action; Gain < 0 for Reverse Action - See Algorithm definition below)
VCONSTANT=v	Valve Constant (Bias) - Fraction open when Error=0 or KC=0 (default=0)

Specification Notes:

The output of each Control Loop must have a destination. Thus, each Control Loop must have either a VID, CLID or PID. In some cases, the Control Loop may have two destinations (e.g., when the output is to be sent to a Valve and to a Multicascade Controller, both VID and CLID would be used).

Inputs (i.e., Measured Values) of Control Loops must have a source. Thus, each Control Loop with Positional algorithm must have a SPID and either a SPUNIT or SPNODE.

The second value in SPVAL=vl,v2 is entered only for a Deadband Controller. In that case, the two values constitute the limits of the dead band.

Specifications (Optional):

NOWINDUP	No windup in Controller (default = Windup allowed)
SPCOMP=	Name, Units, Phase Setpoint Composition Specifications (Required when SPID=COMP)
	Name = Species, Inflow or Base Name (when Base Name is used, such as CO2, refers to same as inflow,. such as CO2IN)
	Units = Composition units
	= WTFR for weight fractions
	= MOLF for mole fraction
	= MOLA for molality
	= GMOL for gmoles
	= GRAM for grams
	Phase = Composition phase
	= TOT for total (all phases combined)
	= LIQ for liquid
	= VAP for vapor
	= SOL for solid
TAUI=v	Integral time (min) (default = 0)
TAUD=v	Derivative time (min) (default = 0)
KCPOLY=A,B,C,D	Variable Gain coefficients - Polynomial form (default=0 for all coefficients) Kc = A + B*MV + C*MV**2 + D/MV MV = Value of Measured Process Variable
KCEXP=A,B,C,D	Variable Gain coefficients - Exponential form (default=0 for all coefficients) Kc = A + B / (C +exp(-D*MV)) MV = Value of Measured Process Variable
DEADTIME=v	Dead Time from process measurement to Output or Stem action (hr) (default = 0)
OLIMIT=v1,v2	Controller Output limits - low limit (v1) and high limit (v2). (default=no limits, except may not result in stem position < 0 or > 1)
CFACTOR=v	Controller Output Factor. When Output is to be sent to another Controller as specified in CLID, the Input to that Controller is the Output from this Controller multiplied times the Controller Output Factor. (default=l)

Specification Note:

The most common use of CFACTOR is when the output of the Control Loop is to be the input to a Multicascade Controller. In that case, the output from this Control Loop may be weighted at some value between 0 and 1, along with the output from other Control Loops providing input to the Multicascade Controller.

Positional Algorithm Definition

Stem Position (Fraction Open) at time j = Stem

$$Stem = Kc\left[\begin{array}{l}\left(ERROR\ (j)\right)\\ \\ +\dfrac{TauD}{60}*\left(\dfrac{(ERROR\ (j)-ERROR\ (j-1)}{TIME\ (j)-TIME\ (j-1)}\right)\\ \\ +\dfrac{60}{TauI}*(\sum ERROR\ (k)*\Delta TIME\ )\end{array}\right]+VConst$$

where:

ERROR(j) = Measured Value - Setpoint Value at time j

Kc = Gain

= Change in Stem Position/Unit Error

When Gain > 0 Direct Action Control

When ERROR is Positive, Stem => 1.0, Open Valve. For Example, Level Control.

When Gain < 0 Reverse Action Control

When ERROR is Positive, Stem => 0.0, Closed Valve. For Example, pH Control of acid waste with NaOH - as pH increases above Setpoint, ERROR is positive and Valve closes.

TauI = Integral time (min)

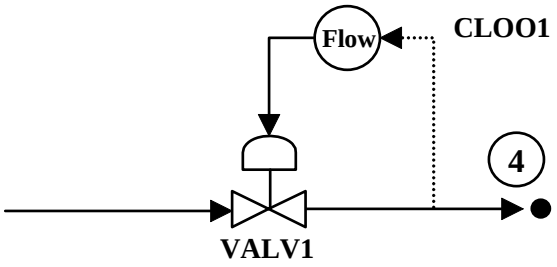
(For NOWINDUP: when Stem Position=1.0 or 0.0, then no addition made to ERROR(k)* TIME)

TauD = Derivative time (min)

VConst = Valve Constant (Bias)

Application 1

A common use of the Positional algorithm is flow control. This case is the same as Velocity algorithm Application 2. Flow at Node 4 will be controlled with a valve (VALV1) immediately preceding it.



The Setpoint will be 5 m^3/hr. The Gain (KC) will be -0.075 (Reverse Acting). The Valve Constant (Bias) will be 0.4, which is the Valve Stem Position when the Error is zero.

CLOO1 VID=1 POSITIONAL SPNODE=4 SPID=FLOW SPVAL=5
KC=0.075 VCONSTANT=0.4

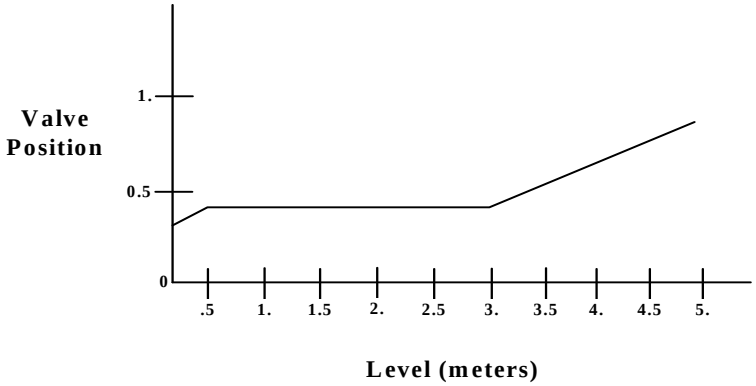
VALV1 DNODE=4 CV=10

Application 2

An effective means of dampening the fluctuations of feed streams is by using a Surge Tank with Deadband Control on the exit. Deadband Control is utilized with the Positional algorithm.

Consider a Surge Tank with several input streams having varying flows and compositions. These inflows will have variable effects on the tank level. The one output stream exits to a process unit in which controllability is important and difficult. That controllability can be enhanced by minimizing the upsets caused by changes in flow exiting the Surge Tank. If the flow is controlled directly by the tank level, the variable nature of the inflows will be transferred to the exit flow. If, however, a range of acceptable levels (Deadband) is defined in which the exit flow will remain constant and the level will be allowed to "float", the fluctuations in exit flow will be eliminated as long as the level is within the "deadband" limits.

Suppose the Surge Tank is to have a maximum level of 5 m. When the level is between 0.5 m and 3 m, the Valve Stem Position on the exit flow will remain at 0.30 (30% open). If the level goes above



3 m the Valve will open under PID Control and if the level goes below 0.5 m, the

Valve will close under PID Control. In this case, the Deadband range is 0.5 to 3 m (SPVAL) and the Deadband Valve Position is 0.30 (VCONSTANT).

The PID Control above and below the Deadband region will utilize a Gain of 0.2 (KC). The Positional algorithm is used with the following qualifications:

1) Below the Deadband region the Error is computed using the lower Deadband limit as the Setpoint.

2) In the Deadband region the Error is set to zero

3) Above the Deadband region the Error is computed using the upper Deadband limit as the Setpoint

The result is as follows:

For Level < 0.5 m Valve Stem Position=0.2 * (Level - *0.5)* + 0.3

For 0.5 < Level < 3 m Valve Stem Position = 0.3

For Level > 3 m Valve Stem Position = 0.2 * (Level - 3.0) + 0.3

The DynaChem Input is as follows:

```
CLOO1    VID=2 POSITIONAL SPUNIT=4 SPID=LEVEL
         SPVAL=0.5,3 VCONSTANT=0.3 KC=0.2
```

Note that the Deadband range is entered as two Setpoint values, the lower first.

SWITCH ALGORITHM

The Switch algorithm is used to fully open a valve at one Setpoint and fully close the valve at another Setpoint. The algorithm may also be used to activate and deactivate a pump in the same manner. Dead Time is optional.

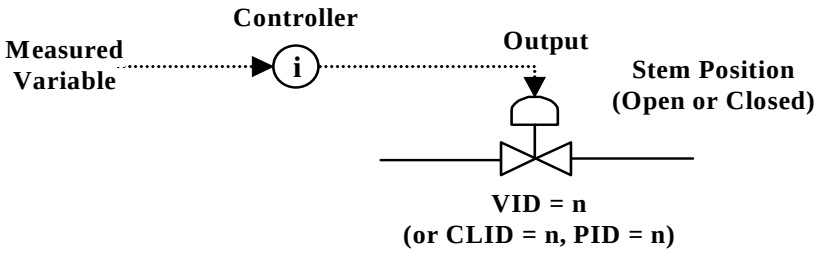
CLOOi SWITCH

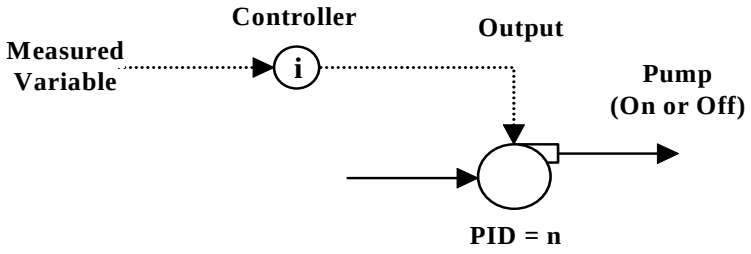
where i represents a unique identification number from 1 to 100.

Specifications (Required):

SWITCH	Switch algorithm (Controller Output = Stem fully open or fully closed)
VID=n	Valve ID to which Control Loop output is to be sent
CLID=n	Control Loop ID to which Control Loop output is to be sent
PID=n	PUMP ID to which Control Loop output is to be sent
SPUNIT=n	Setpoint Unit ID (used with SPID=TENT, PRES, PH, LEVEL or COMP)
SPNODE=n	Setpoint Node ID (used with SPID=TEMP, PRES, PH FLOW or COMP)

SPID=a	Setpoint Value ID SPID = TEMP for Temperature (°C) SPID = PRES for Pressure (atm) SPID = PH for pH SPID = LEVEL for Level (m) (may not be used with SPNODE) SPID = FLOW for Flow (m^3/Hr) (may not be used with SPUNIT) SPID = CONT for Composition (SPCOMP also required)
OPEN=v	Setpoint at which Stem is opened fully
CLOSE=v	Setpoint at which Stem is closed fully





Specification Notes:

The output of each Control Loop must have a destination. Thus, each Control Loop must have either a VID, CLID or PID. In some cases, the Control Loop must have two destinations (e.g., when the output is to be sent to a Valve and a Multicascade Controller, both VID and CLID would be used).

Inputs (i.e., Measured Values) of Control Loops must have a source. Thus, each Control Loop with Switch algorithm must have a SPID and either a SPUNIT or SPNODE.

Specifications (Optional):

SPCOMP=	Name, Units, Phase Setpoint Composition Specifications (Required when SPID=COMP) Name = Species, Inflow or Base Name (when Base Name is used, such as CO2, refers to same as inflow, such as CO2IN) Units = Composition units = WTFR for weight fraction

= MOLF for mole fraction
= GMOL for gmoles
= GRAM for grams

Phase = Composition phase
= TOT for total (all phases combined)
= LIQ for liquid
= VAP for vapor
= SOL for solid

DEADTIME=v Dead Time for process measurement to Output or Stem action (hr)(default = 0)

CFACTOR=v Controller Output Factor. When Output is to be sent to another Controller as specified in CLID, the Input to that Controller is the Output from this Controller multiplied times the Controller Output Factor. (default=1)

Specification Note:

The most common use of CFACTOR is when the output of the Control Loop is to be the input to a Multicascade Controller. In that case, the output from this Control Loop may be weighted at some value between 0 and 1, along with output from other Control Loops providing input to the Multicascade Controller.

Switch Algorithm Definition

At the Setpoint (defined by SPUNIT/SPNODE, SPID, SPCOMP) becomes equal to the specified Open Value (OPEN) the controller output is set to 1. As the Setpoint value becomes equal to the specified Close Value (CLOSE) the controller output is set to 0.0.

When Measured Value = Open Value then Controller Output = 1

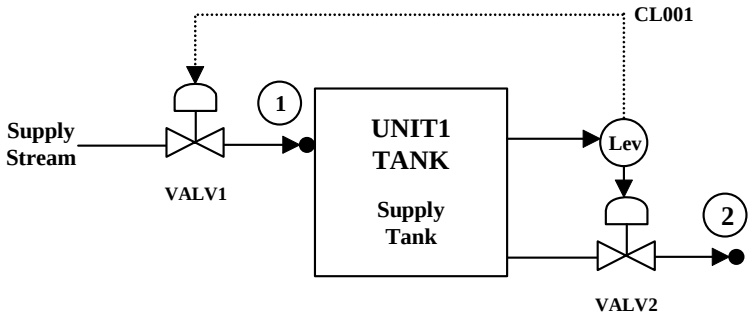
When Measured Value = Close Value then Controller Output = 0

When the output destination is a Valve (VID), the output is applied as a Valve Stem Position.

When the output destination is a Pump (PID), the output is applied as the Pump Speed Override (Fraction of Maximum Pump Speed).

Application I

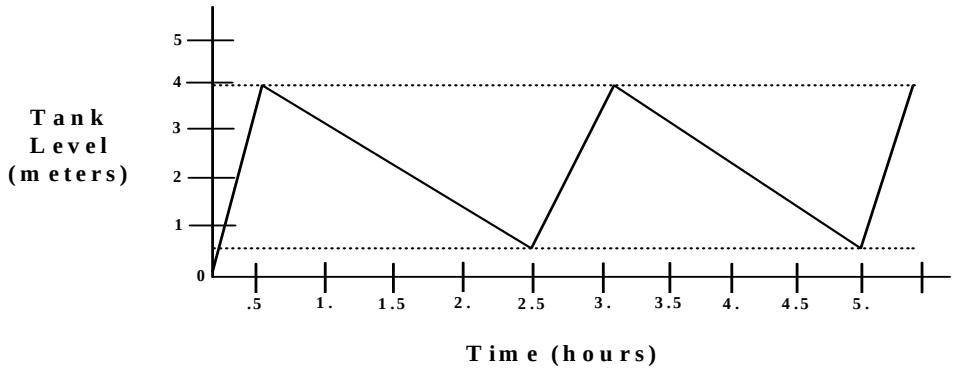
A Supply Tank exit is being used to meter fluid into another process unit in a continuous mode. The Supply Tank is refilled by the Supply Stream whenever necessary to maintain a minimum level of 0.5 meter. The Switch algorithm may be used in a feedback controller to fill the Supply Tank as needed. For simplicity, the upstream Supply Stream source (an ENTRY or a TANK) and the downstream destination of the metered fluid (a TANK) will be omitted.

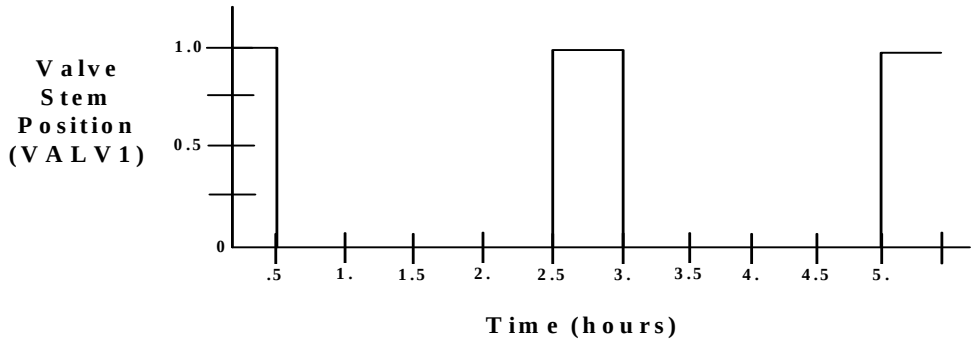


The Supply Tank (UNIT1) will be replenished by the Supply Stream (Node 1) when the level reaches 0.5 m. The Supply Tank will be refilled to a level of 4 m and the Supply Stream valve (VALV1) will be closed until the level reaches 0.5 m again. Assuming the Supply Tank is empty initially, the Supply Stream must be started manually (VOPEN=1). The exit line will be closed initially until sufficient fluid has been supplied to the tank. The DynaChem Input is as follows:

```
VALV2     DNODE=2 CV=10
VALV1     DNODE=1 CV=100 VOPEN=1
CLOO1     VID=1 SWITCH SPUNIT=1 SPID=LEVEL
          OPEN=0.5 CLOSE=4
```

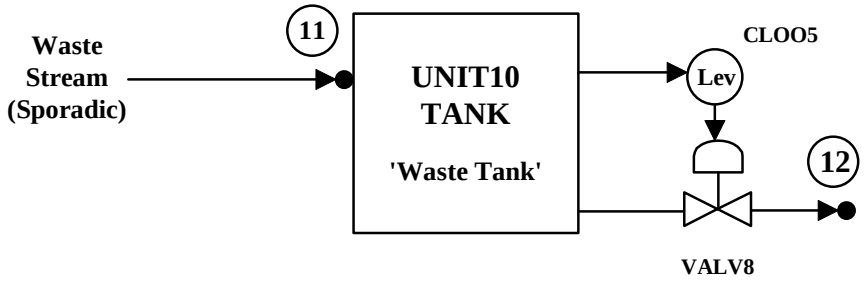
Plots of the resulting tank level and Valve Stem Position (fraction open) will have the following form:





Application 2

A Waste Tank will accept sporadic deliveries of fluid. When sufficient fluid has accumulated, a batch will be removed for processing.



The Waste Tank will have a diameter of 3 m (CSA=7.07 m^2) and a Maximum Level of 6 m. It will be desirable to maintain a minimum fluid level of 1 m in the tank.

The minimum batch size to be sent to processing will be 20 m^3. If 1 m of fluid is to remain in the tank, there will be sufficient fluid for a batch to be withdrawn when the level reaches 3.83 m (20 m^3 / 7.07 m^3 + 1 m). Thus, the valve should open when the level reaches 3.83 m and close again when the level reaches 1 m.

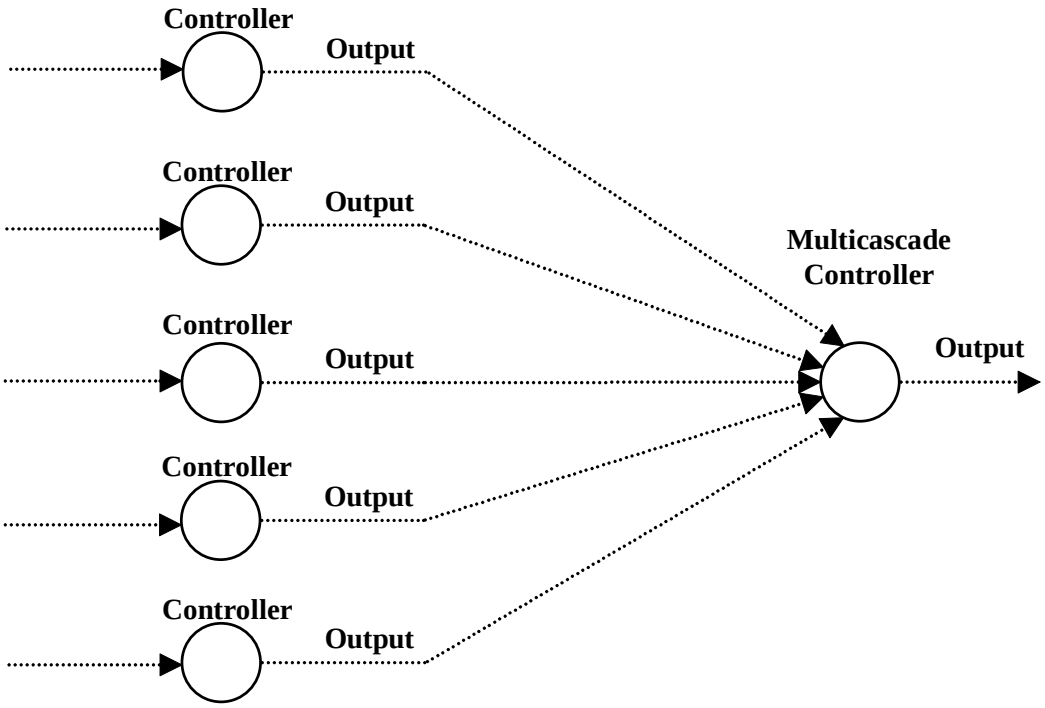
UNIT10	TANK 'WASTE TANK' UNODE=11 DNODE=12
	CSA=7.07 MAXLEVEL=6
VALV8	DNODE=12 CV=50
CLOO5	VID=8 SWITCH SPUNIT=10 SPID=LEVEL
	OPEN=3.83 CLOSE=1

MULTICASCADE ALGORITHM

The Multicascade algorithm (1) acquires the output from 1 to 5 other controllers, (2) applies the Output Factors specified for those controllers, (3) sums the factored outputs, and (4) applies the resulting output as a Valve Stem Position change. Thus, the output of a Multicascade Controller is applied as a Velocity Controller is applied, as a ΔStem.

Dead Time and Output Limits are optional.

Schematic:



CLOOi MULTICASCADE

where i represents a unique identification number from 1 to 100.

Specifications (Required):

MULTICASCADE	Multicascade algorithm (Controller Output = Sum of up to 5 Factored Stem movements determined by other Control Loops)
VID=n	Valve ID to which Control Loop output is to be sent

Specification note:

Inputs of Control Loops must have a source. Multicascade inputs come from Control Loops having a CLID entry specifying the Multicascade Control Loop as its destination.

Specifications (Optional):

DEADTIME=v	Dead Time from process measurement to Output or Stem action (hr) (default = 0)
OLIMIT=v1,v2	Controller Output limits - low limit (v1) and high limit (v2). (default=No limits, except may not result in stem position < 0 or > 0

Specification Note:

The Output Limits shown here are for the Multicascade Output. If Output Limits are to be placed on the Inputs to the Multicascade Control Loop, they should be entered with the Control

Loop producing the Output.

Multicascade Algorithm Definition

Stem Movement at time j = Stem

= Stem Fraction Open at time j

- Stem Fraction Open at time j-1

Note: Stem may not result in a Stem Position less than 0 or greater than 1.

Stem = Factor(l)* Stem(l) + Factor(2)* Stem(2) + Factor(3)* Stem(3) + Factor(4)* Stem(4)+Factor(5)* Stem(5)

where Stem = Stem Movement at time j from Multicascade Controller

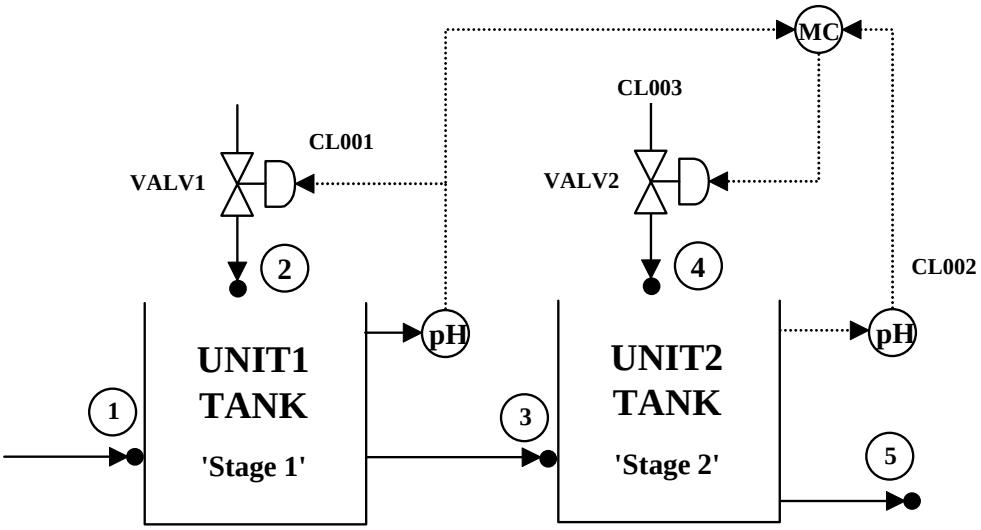
Stem(i) = Stem Movement at time j from Control Loop i

Factor(I) = Output Factor from Control Loop I

Application 1

A two-stage neutralization process will use a Multicascade Controller to provide the 2nd stage with feedforward assistance from Stage 1.

A pH Control Loop (CLOO1) will measure the pH in Stage 1 (UNIT1) and control the pH in that stage at 3 using Valve 1. The Output from that Loop will also be sent to the Multicascade Control Loop (CLOO3). The other input to the Multicascade Control Loop will be from a pH Control Loop (CLOO2) on Stage 2 (UNIT2) with a pH setpoint of 9. This pH Control Loop, however, will send output to the Multicascade Control Loop only. The valve controlling the reagent flow to Stage 2 (VALV2) will be controlled not by the pH Control Loop, but by the Multicascade Controller (CLOO3). Thus, as an upset requires additional reagent in Stage 1, this information will feed forward to Stage 2 in anticipation of the upset.



The two inputs to the Multicascade Controller will be factored as follows:

Time = 0 to 0. 1 hour	CLOO1 Output Factor = .8
	CLOO2 Output Factor = .2
Time = 0. 1 to end	CLOO1 Output Factor = .*5*
	CLOO2 Output Factor = .*5*

Thus, initially the upstream stage (UNIT1) will dominate the control in Stage 2. This will reduce startup fluctuations seen in Stage 2 by predicting them. After the initial startup period of 0.1 hour, each controller will contribute half of the Valve Stem Movement in Stage 2. In this case, the factors add to unity, which is not necessary.

CLOO1	VID=1 CLID=3 SPUNIT=L SPID=PH SPVAL=3
	KC= -0.0l TAUI=0.5
	CFACTOR=0.8 CFACTOR=0.5 (TIME=0.1)
CLOO2	CLID=3 SPUNrr=2 SPID=PH SPVAL=9
	CFACTOR=0.2 CFACTOR=0.5 (TIME=0.l)
	CLOO3 VID=2 MULTICASCADE
	VALV1 DNODE=2 CV=20
	VALV2 DNODE=4 CV=30

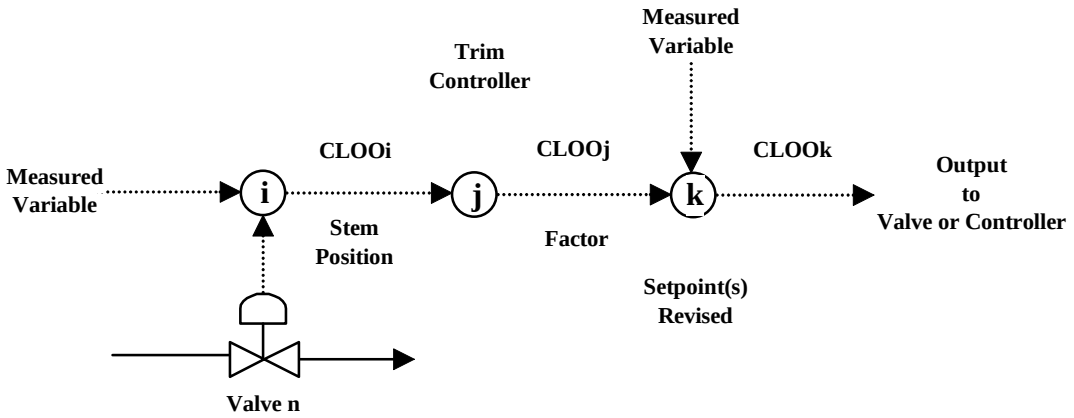
TRIM ALGORITHM

The Trim algorithm revises the Setpoint value(s) of another controller based upon the Stem

Position of the valve. The Trim Controller

1) Is supplied to the Stem Position of a valve by the Controller which controls the valve
2) Compares the Stem Position to the specified Trim limits
3) Computes a Factor based upon the comparison made in step 2
4) Applies the computed Factor to the Setpoint value(s) of a specified Control Loop

Schematic:



CLOOj TRIM=s1, s2

where j represents a unique identification number from 1 to 100.

Specifications (Required):

TRIM=s1,s2	Trim Controller algorithm with Emits of s1 to s2
CLIID=k	Control Loop BD to which Control Loop output is to be sent (Control Loop containing Setpoint value(s) to be revised)
KC=v	Gain (default = 0)

Specifications (Optional)

KCPOLY=A,B,C,D	Variable Gain coefficients - Polynomial form (default=0 for all coefficients) Kc = A + B*MV + C*MV**2 + D/MV MV = Value of Measured Process Variable
KCEXP=A,B,C,D	Variable Gain coefficients - Exponential form (default=0 for all coefficients) Kc = A + B / (C + exp(-D*MV)) MV = Value of Measured Process Variable

DEADTIME=v	Dead Time from process measurement to Output or Stem action (hr)(default = 0)
OLIMIT=v1,v2	Controller Output limits - low limit (v1) and high limit (v2). (default=No limits, except may not result in stem position <0 or > 1)
CFACTOR=v	Controller Output Factor. When Output is to be sent to another controller (as specified in CLID) the Input to that controller is the Output from this Controller multiplied times the Controller Output Factor. (default=1)

A Trim Control Loop requires three controllers (see diagram above):

1) The Control Loop which supplies the Valve Stem Position (Control Loop i)

   CLOOi CLID=j VID=n...

2) The Control Loop containing the Trim Controller (Control Loop j)

   CLOOj CLID=k TRIM=s1,s2 KC=v...

3) The Control Loop whose Setpoint is to be adjusted (Control Loop k)

   CLOOk SPVAL=v...

The Stem Position of Valve n is used as the Measured Variable in the Trim Controller (CLOOj).

The ERROR is computed based upon the Trim Limits (s1,s2).

If Stem Position < s1 then ERROR = Stem - s1

If s1 $\leq$ Stem Position $\leq$ s2 then ERROR = 0

If s2 < Stem Position then ERROR = Stem - s2

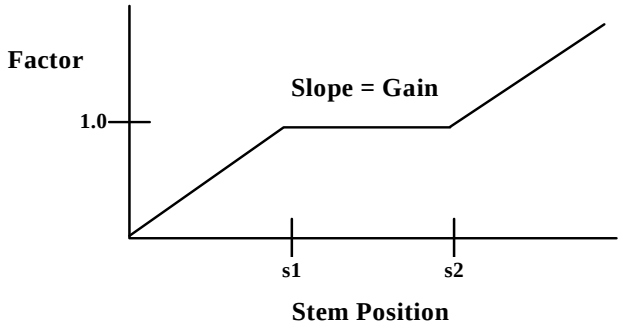
The computed Factor is

Factor = 1.0 + ERROR * KC

The Factor is then multiplied times the Setpoint Value(s) of the Control Loop to be adjusted (CLOOk). Furthermore, the Factor is applied to the following values as well:

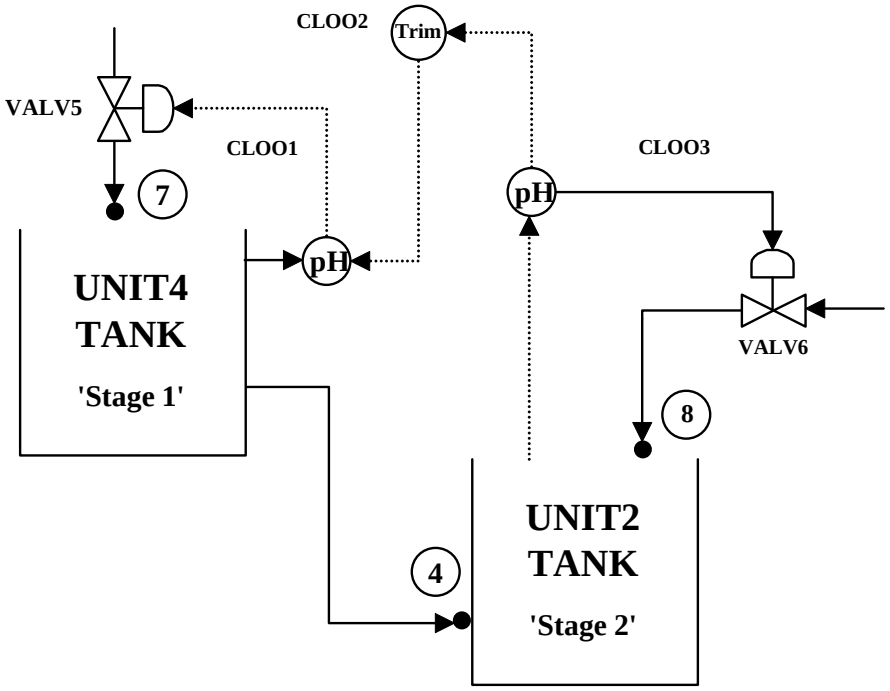
1) Both low and high Setpoints for Deadband Control
2) Both Open and Close values for Switch
3) Ratio value for Ratio Control

Notice that when Stem < s1, the ERROR is negative and when Stem > s2, the ERROR is positive. The sign of the Gain (KC) should be chosen appropriately. For example, suppose you want to decrease the setpoint of CLOOk when Valve n is closed (and, therefore, less than s1). The functional representation of STEM versus Factor is shown below. In order to achieve this result, KC should be positive.



Application 1

In the Two Stage Neutralization shown below it is desired to decrease the Setpoint in Stage 1 (CLOO1) when the valve on the Reagent Flow (VALV6) is closed. That is, the valve being closed is interpreted as meaning that too much neutralization is being accomplished in Stage 1 resulting in no action required by Stage 2. Thus, the Setpoint in Stage 1 is made more acidic requiring less neutralization. Similarly, if the valve is open too much it means the Setpoint in Stage 1 is too low and should be raised to result in more neutralization before reaching Stage 2.



The Valve Stem Position of the reagent stream to the 2nd Stage Neutralization tank (VALV6, Controlled by CLOO3) is compared to Trim Limits of 0.15 and 0.4 (specified in CLOO2). The Factor is then computed with Limits of 0.75 and 1.2 (OLIMIT=0.75,1.2) which means that the Factor itself cannot be less than 0.75 or greater than 1.2. OLIMIT applies only to the Factor, not to the resulting Setpoint value(s).

In computing the Factor,

1) When the Valve Stem (VALV6) is open less than .15, the feed to Stage 2 is judged to be

2) too alkaline for good control. Therefore, the pH Setpoint for the 1st stage is lowered to reduce the neutralization carried out in Stage 1.

3) When the Valve Stem (VALV6) is open greater than .4, the feed is judged to be too acidic and the pH Setpoint in Stage 1 is increased.

4) If the Step Position (VALV6) is between .15 and .4, it is judged that the feed to Stage 1 is within the range of the 2nd Stage's controllability and the pH Setpoint is left unchanged (Factor=1).

The Factor is applied to the Setpoint Value (pH) of the Control Loop controlling reagent flow to the 1st Stage (CLOO1). Since the Factor is multiplied times the current Setpoint Value, an initial value must be included (SPVAL=2).

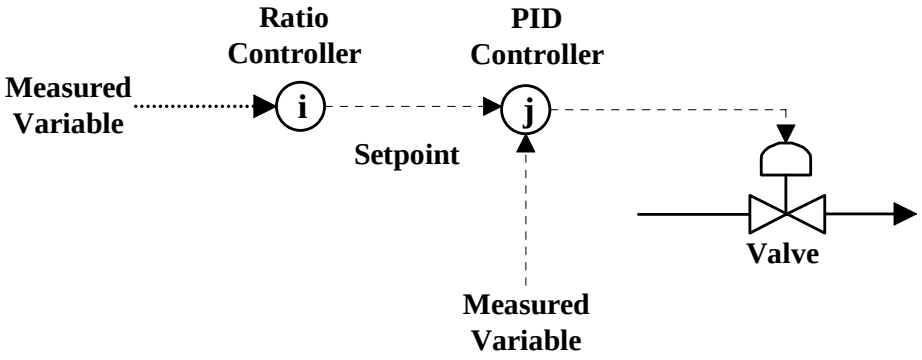
The DynaChem Input is as follows:

```
CLOO3     VID=6   CLID=2   SPUNIT=5   SPID=PH   SPVAL=9
          KC= -0.ll   TAUI=1
CLOO2     CLID=1   TRIM=0.15,0.4 KC=0.05
          OLIMIT=0.75,1.2
CLOO1     VID=5 SPUNIT=4 SPID=PH SPVAL=2
          KC= -0.0l TAUI=0.5
```

RATIO Algorithm

The Ratio algorithm acquires the value of a specified measured variable, multiplies that value times a specified factor (Ratio) and uses the result to replace the Setpoint of another control Loop. Thus, the second Control Loop becomes "ratioed" to the first Control Loop.

Schematic:



CLOOi RATIO=v

where i represents a unique identification number from 1 to 100.

Specifications (Required):

RATIO=v — Ratio Control algorithm with a ratio value of v (Controller output = Ratio * Measured Value)

CLID=j — Control Loop ID to which Control Loop output is to be sent (Control Loop containing Setpoint value to be revised)

SPUNIT=n — Measured Variable Unit ID (used with SPID=TEMP, PRES, PH, LEVEL or COMP)

SPNODE=n — Measured Variable Node ID (used with SPID=TEMP, PRES, PH, FLOW or COMP)

SPID=a — Measured Variable Value ID

- SPID = TEMP for Temperature °C)
- SPID = PRES for Pressure (atm)
- SPID = PH for pH
- SPID = LEVEL for Level (m) (May not be used with SPNODE)
- SPID = FLOW for Flow (m^3/Hr) (May not be used with SPUNIT)
- SPID = CONT for Composition (SPCOMP also required)

Specification Notes:

Inputs (i.e., Measured Value) of Control Loops must have a source. Thus, each Ratio Control

Loop must have a SPID and either a SPUNIT or SPNODE.

For a Ratio Controller, SPUNIT, SPNODE and SPID are the same as a SPVAL case, except they refer to the Measured Variable, not actually to a Setpoint.

Specifications (Optional):

SPCOMP= — Name, Units, Phase, Setpoint Composition Specifications
(Required when SPID=COMP)

Name = Species, inflow or base Name (when Base Name is used, such as CO2, refers to same as inflow, such as CO2IN)

Units = Composition units

- = WTFR for weight fraction
- = MOLF for mole fraction
- = MOLA for molality
- = GMOL for gmoles
- = GRAM for grams

Phase = Composition phase

- = TOT for total (all phases combined)
- = LIQ for liquid
- = VAP for vapor
- = SOL for solid

DEADTIME=v	Dead Time from processed measurement to Output or Stem action (hr)(default=0)
OLIMIT==v1,v2	Controller output limits - low limit (v1) and high limit (v2). (default=No limits, except may not result in stem position < 0 or > 1)
CFACTOR=v	Controller Output Factor. When Output is to be sent to another Controller (as specified in CLID) the Input to that controller is the Output from this Controller multiplied times the Controller Output Factor. (default=1)

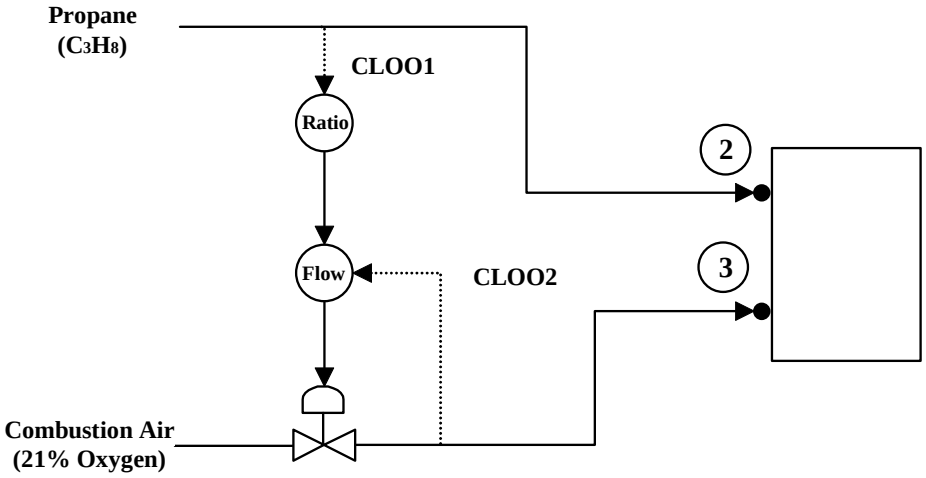
Ratio Algorithm Definition

If Control Loop i employs the Ratio algorithm and Control Loop j is the destination:

Setpoint of Control Loop j = Measured Variable of Control Loop i * Ratio Value of Control Loop i

Application 1

The combustion airflow to a propane burner is to be controlled with a Ratio Controller.



The Combustion reaction is carried to completion:

C3H8 + 5 O2 => 3 CO2 + 4 H2O

The combustion air should contain 20% excess (molar basis).

Air, of course, is 21% oxygen (molar basis). Thus:

$$\frac{\text{Air (gmole)}}{\text{C3H8 (gmole)}} = \frac{5\text{gmole CO2}}{1\text{ gmole C3H8}} * 1.2 * \frac{1\text{ gmole Air}}{0.21\text{ gmole O2}} = 28.6$$

Since both gas streams are at the same temperature and pressure and the delivery pressure is low, the Ideal Gas Law shows that the molar ratio is also the volumetric ratio. Therefore, the ratio of the volumetric flow of the Air stream to the Propane stream is 28.6.

The Ratio Control Loop (CLOO1) measures the flow of the Combustion gas (Node 2), multiplies it times 28.6 (RATIO) and uses the result as the Setpoint in the Air Stream Flow Control Loop (CLOO2). The Air Stream Flow Control is simply a Velocity algorithm, Reverse Acting PID Controller. It differs from other such controllers only in that its Setpoint is being set dynamically by the Ratio Controller. Notice that a Setpoint of 2.1 was used to initiate Control Loop 2.

The DynaChem Input is as follows:

```
CLOO1    CLID=2 RATIO=28.6 SPNODE=2 SPID=FLOW
CLOO2    VID=4 SPNODE=3 SPID=FLOW SPVAL=2.1
         KC= -0.l TAUI=1
```

DEAD TIME

Dead Time is the time period between (1) computation of the Controller Output based upon the current parameters (e.g., Setpoint, Measured Variable value, Gain) and (2) application of the Output to the appropriate Valve or Control Loop. Dead Time may be applied to any Control Loop.

```
CLOOi    DEADTIME=v
```

The Dead Time (v) is in hours. The maximum allowable value is 10 times the system time increment (TINC). The default value is zero, in which case the output is applied immediately. There is, however, Implicit Dead Time inherent in some process configurations (See Implicit Dead Time).

The procedure for applying Dead Time is as follows. The Controller computes Error and Output at each time step. The Output is saved and applied to the Valve or another Controller (e.g., Multicascade Controller) v hours later. In the case of a Ratio Controller, the revised Setpoint is also set v hours later. The following is a hypothetical case to describe the application of Dead Time:

Setpoint ID = pH Setpoint Value = 9

Time Increment = 0.01 hour Dead Time = 0.015 hour

Initial Valve Stem Position = 0

Velocity Algorithm, Kc=-0.l, TauI=0, TauD=0:

Delta Stem = -0.1 * (Err(n) - Err(n-1))

Columns 1, 2, 3 and 4 on the following page (Time, pH, Error and Output) are all computed t he same regardless of Dead Time. When Dead Time = 0 (default) the Input to the valve is identical to the Controller Output at the time increment. In this case, however the Dead Time (0.015 hour) causes the Output to be delayed by 1.5 time increments before it is applied as Input to the valve. Column 5 shows the reference time for the Output reaching the valve as Input (Time - Dead Time). Column 6 shows the valve Input and Column 7 the resulting Stem Position.

When Dead Time is not an integral of the time increment, the Input to the valve Output is a composite of controller Output from two time increments. The Output from the controller begins at the specified time (computation time) and remains in effect until the next time increment begins.

1	2	3	4	5	6	7
Time	Measured pH	Error	Output (Stem Movt)	Ref Time (Time-Dead)	Input (Stem Movt)	Valve Stem
.00	7.1	-1.9	--	0	0	0
.01	7.1	-1.9	--	0	0	0
.02	5.2	-3.8	0.19	0.005	0	0
.03	4.0	-5.0	0.12	0.015	0.095	0.095
.04	3.2	-5.8	0.08	0.025	0.155	0.250
.05	2.9	-6.1	0.03	0.035	0.100	0.350
.06	3.1	-5.9	-0.02	0.045	0.055	0.405
.07	5.5	-3.5	-0.24	0.055	0.005	0.410
.08	7.6	-1.4	-0.21	0.065	-0.130	0.280
.09	10.2	1.2	-0.26	0.075	-0.225	0.055
.10	12.1	3.1	-0.19	0.085	-0.235	0
.11	11.8	2.8	0.03	0.095	-0.225	0
.12	11.5	2.5	0.03	0.105	0.015	0.015
.13	11.0	2.0	0.05	0.115	0.030	0.045

For example, in the case above, at time 0.04, the reference time 0.025. The valve Input for time = 0.04 to 0.05 will be the Controller Output from 0.025 to 0.035. At time = 0.02, the Controller Output is computed as 0.19 and remains that value until time = 0.03 when it becomes 0.12. Therefore, from time 0.025 to 0.035, the Controller Output was 0. 19 for 0.005 hour and 0.12 for 0.005 hour. These Output are applied as Input to the valve in order and weighted according to the time in effect. The Input to the valve will be in two steps:

Initial Valve Stem Position (at time = 0.03) 0.095

Valve Input 1: $0.19 * \frac{(0.030-0.0251)}{(0.030-0.020)} = 0.095$

Resulting Valve Stem Position = 0.095 + 0.095 = 0.190

Valve Input 2: $0.12 * \frac{(0.035-0.030)}{(0.040-0.030)} = 0.060$

Resulting Valve Stem Position = 0.190 + 0.060 = 0.250

From time 0.04 to 0.05 the Total Input to the valve is 0.155 (Valve Input 1 + Valve Input 2). For this time increment, the resulting Input is the weighted average of the Output during the Reference time. This is not, however, always the case.

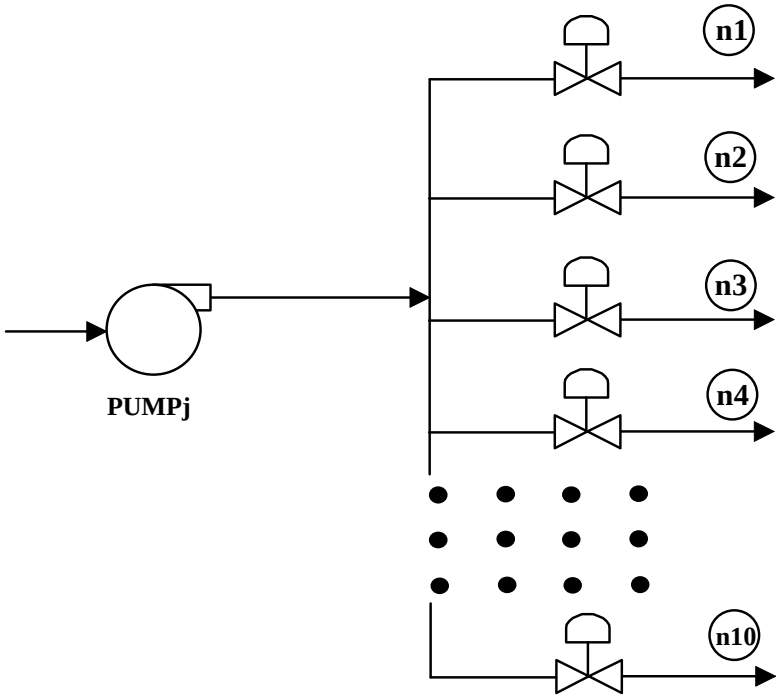
At time = 0.12, the Reference time is 0. 105. The Output from time 0. 105 to 0.11 is -0.19 and from time = 0.11 to 0.115, the Output is 0.03. Thus,

Initial Valve Stem Position (at time = 0.11) = 0.0

Chapter 6: PUMP SPECIFICATION

A Pump is used to increase fluid (liquid + suspended solid) pressure. The flow, pump speed and User specified Pump Curves are used to determine the Developed Head. The Developed Head is used with the suction head, suction pressure drop and pump elevation to compute the pump discharge pressure.

One Pump may be associated with up to 10 Downstream Nodes all of which must be DNODE



entries of the same Unit. Valves are optional.

PUMP j

where j represents a unique identification number from 1 to 50.

Specifications (Required):

DNODE=n,...	Downstream Node Number(s) - minimum for Pump is 1 and maximum is 10.
PELEV=v	Pump elevation with reference to tank zero level (can be negative). (Default = 0)
PSPEED=v	Pump maximum speed (rpm)
PSDROP=A,B,C	Pump suction pressure drop coefficients: Pres Drop (m H20)

	=A*(Flow**2) + B*Flow + C (Flow in m^3/hr) (default: A=0, B=0, C=0)
PCURV=S,F1,H1,F2,H2...	Pump Curve for speed S (rpm) Fl=lst Flow (m^3/hr) Hl=lst Head (m H20) F2=2nd Flow (m^3/hr) H2=2nd Head (m H20) : : : : : : : :

Specification Notes:

For PCURV Keyword may be used multiple times in a PUMP, once for each Speed. The maximum number of curves per pump is 20.

There is no limit to the number of points in any single Pump Curve. The total number of entries (including S,F1,Hl each as 1 entry) for all combined Pump Curves in the entire model may not exceed 500.

Specifications (Optional):

PSWITCH=V	Pump speed override (Fraction of pump maximum speed) (default=1)

Pump Algorithm Definition

The following values are supplied to the Pump computation:

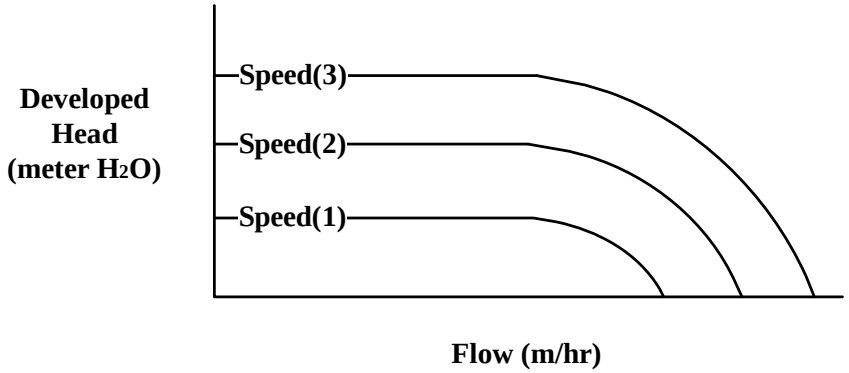
SPEED = Pump speed (rpm) = Maximum Pump Speed * Pump Speed Override

FLOW = Total fluid through pump (m^3/hr) = Sum of flows placed at all Downstream Nodes associated with the Pump.

PSUCT = Suction Pressure (m H20) = Upstream Unit Pressure + Fluid Height.

PELEV = Pump elevation with respect to Unit zero level (m)

Pump Curves:



A series of coordinates is entered using the Keyword PCURV to define each Pump Curve. Up to 20 Curves may be entered for a Pump. The values entered for Pump Curve i are:

Speed(i), Flow(i,1), Head(i,1), Flow(L2), Head(i,2)....

The Pump discharge pressure is computed as follows:

1) Compute the Developed Head.

Determine Pump Curve i having Speed (i) $\leq$ SPEED and Pump Curve j win have Speed(j) > SPEED. Thus, the Pump Speed (SPEED) lies between curves i and j.

$$\text{Sfactor} = \frac{\text{SPEED - Speed(i)}}{\text{Speed(j) - Speed(i)}}$$

If the Pump Speed is less than the lowest Speed(i), then the lowest Speed Curve is used and SFactor=0. If the Pump Speed is greater than the highest Speed(i), then the highest Speed Curve is used and SFactor = 0.

For Curve i, determine the Flow(i,1) $\leq$ FLOW and Flow(I,2) > FLOW. Thus, the Flow (FLOW) lies between points Flow(i,1) and Flow(i,2). The Developed. Head associated with each of those flows are Head(i,1) and Head(i,2), respectively.

$$\text{FFactor(i)} = \frac{\text{FLOW - Flow(i,1)}}{\text{Flow(i,2) - Flow(i,1)}}$$

Head(i) = Head(i,1) + FFactor(i) * (Head(i,2) - Head - Head(i,1))

For Curve j, compute the same:

$$\text{FFactor(j)} \quad \frac{\text{FLOW - Flow(i,1)}}{\text{Flow(j,2) - Flow(j,1)}}$$

Head(j) = Head(j,1) + FFactor(j) * (Head(j,2) - Head(j,1))

Head(i) and Head(j) are the interpolated values for the Developed Head for Speed(i) and

Speed(j), respectively, at a fluid flow of FLOW. Interpolation for Speed is computed as

HEAD = Developed Head (m H20)
= Head(i) + SFactor * (Head(j) - Head(i))

2) Compute the Suction Pressure Drop.

PSDROP = Suction Pressure Drop (m H20)
= A * FLOW**2 + B * FLOW + C

3) Compute Pump Discharge Pressure

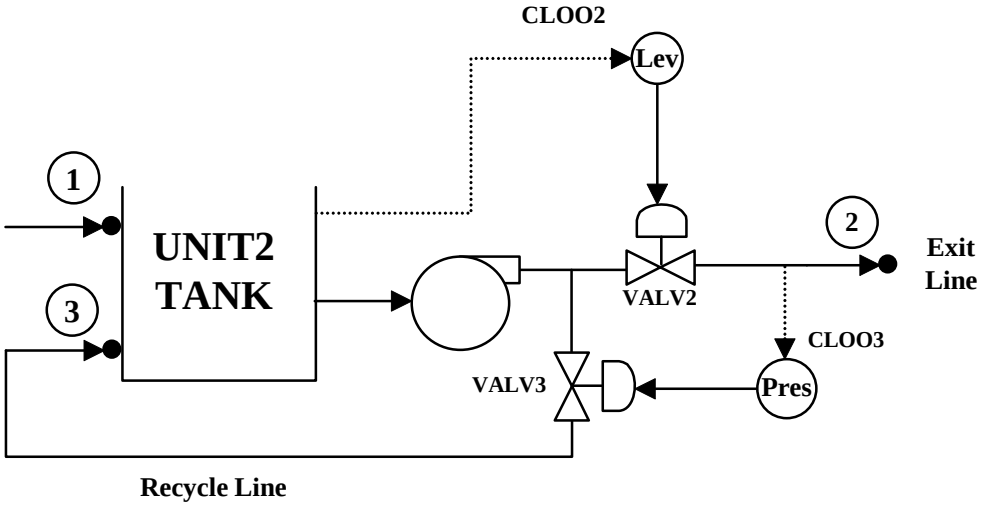
PDIS = Pump Discharge Pressure (m H20)
= PSUCT - PELEV - PSDROP + HEAD

PDISA = Pump Discharge Pressure (atm)
= PDIS / 10.34

Application 1

A tank recycle line will be used to maintain constant pressure on a pump discharge from a tank exit.

A Pump (PUMP1) will be placed on the exit line of a Tank (UNIT2). Two lines (Exit Line and Recycle Line) will branch at the Pump Discharge. The tank level will be controlled at 1 meter by a control loop (CLOO2) adjusting the flow through a valve (VALV2) on the Exit Line. The discharge pressure will be controlled at 2 atm by a control loop (CLOO3) adjusting the flow through a valve in the Recycle Line (VALV3). The discharge pressure will be measured at Node 2.



Three Pump Curves will be entered:

Speed = 500 rpm		Speed = 750 rpm		Speed = 1000 rpm	
Flow (m^3/hr)	Head (m H20)	Flow (m^3/hr)	Head (m H20)	Flow (m^3/hr)	Head (m H20)
0	15	0	33.7	0	60
2.8	15	4.2	33.75	5.6	60
5	12	5	31	9	55
7	7.5	8.6	25	12	47.5
9	2.5	11	17.5	15	37.5
10	0	12.9	10	17.4	25
		15	0	19	13
				20	0

The Pump suction line will exit. the Tank at the zero level and drop 0.1 meter to the Pump (PELEV). The discharge from the Pump splits to form the Exit and Recycle Lines. Both lines are entered as having an exit level of zero (LEXIT=0,0) which is the default and need not be entered.

The maximum Pump Speed (PSPEED) will be 1000 RPM and the Pump Speed Override (PSWITCH) will be set at 0.8 so that the effective pump speed will be 800 RPM. The Suction Pressure Drop coefficient (PSDROP) will be 0.02 (i.e., Pressure Drop = 0.02 Flow**2).

The DynaChem Input File is as follows:

```
NODE ORDER=1,2

UNIT      TANK UNODE=1,3 DNODE=2,3 CSA=5 MAXVOL=15 STATE=90,1
VALV2     DNODE=2 CV=40
VALV3     DNODE=3 CV=20
CLOO2     VID=2 SPUNIT=2 SPID=LEVEL SPVAL=1 KC=0.15 TAUI=1
CLOO3     VID=3 SPNODE=3 SPID=PRES SPVAL=2 KC=0.04 TAUI=0.5
PUMP1     DNODE=2,3 PELEV=-0.l SPSEED=1000 PSWTICH=0.8 PSDROP=0.02
          PCURV=500, 0,15, 2.8,15, 5, 12, 7,7.5, 9,2.5, 10,0
          PCURV=750, 0,33.75, 4.2,33.75, 6,31, 8.6,25,11,17.5, 12.9,10,15,0
          PCURV=1000, 0,60, 5.6,60, 9,55, 12,47.5, 15,37.5,17.4,25, 19,13, 20,0
```

Chapter 7: NODE SPECIFICATION

The NODE Keyword is used to specify the order in which Nodes, and hence all other computations, are completed.

NODE ORDER=nl,n2,...

Specifications (Required):

NODE=nl,n2,... Order in which Nodes are to be computed each time increment.

Specification of Node Order determines the order in which all computations are completed. Specification of a Node results in the computation of the following:

1) The Unit directly upstream from the Node (i.e., the Unit for which the Node is a DNODE entry)
2) All Nodes in the DNODE list for that Unit
3) All Valves associated with all Nodes in (2)
4) All Pumps associated with the Valves in (3)
5) All Control Loops associated with the Valves in (3)
6) All Control Loops associated with Control Loops in (5)

Thus, specification of a Node in the Node Order results in the computation of all associated Units, Valves, Pumps and Control Loops.

The selection of Node Order may result in Implicit Dead Time in the model and should be considered when defining Order (See Implicit Dead Time).

IMPLICIT DEAD TIME

When a Controller's Measured Value is the Level of the same Unit to which the valve is attached (Figure 1) or the Flow at the Node associated with the valve (Figure 2), the Measured Value is acquired at the beginning of the Unit computation and is, therefore, the final value from the previous time step.

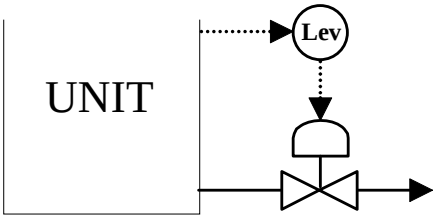


Figure 1

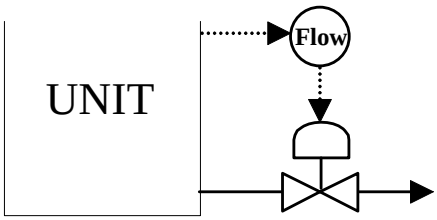


Figure 2

As a result, there is Implicit Dead Time equivalent to one system time increment. This phenomenon does not apply to the intensive properties of temperature, pressure and pH. The Measured Value for these properties are determined at the end of the unit computation and, therefore, no Implicit Dead Time is included.

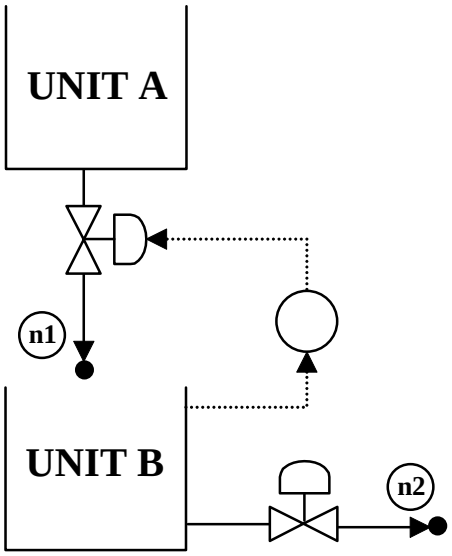


Figure 3

When two Units are involved in a Control Loop (Figure 3), Implicit Dead Time results if the Unit with the associated Valve (Unit A) is computed before the Unit with the Measured Variable (Unit B). This phenomenon is accomplished through the NODE ORDER list.

No Implicit Dead Time: NODE ORDER=N2,N1

Implicit Dead Time equivalent to One System Increment: NODE ORDER=N1,N2

Chapter 8: TIME SPECIFICATION

The TIME Keyword is used to set the length of the simulation and the time increment (time step size).

TIME TEND=t1 TINC=t2

Specifications (Required):

TEND=t1 End time (hr) (default=0; only the initial conditions are computed)
TINC=t2 Time increment (hr)

Since Interactive cases may be terminated whenever desired, the End Time should be made suitably high to allow the simulation to run for the necessary length. If, however, the User intends to interrupt an Interactive run, it should be remembered that the SAVE capability default is to write a Restart file at the end of the run only. Therefore, when entering a high value for End Time with the intention of interrupting before reaching the Time, the SAVE Keyword should be used to save the Restart file at a reasonable frequency.

The objective of DynaChem is to represent an "analog" process with a "digital" and, therefore, discrete model. The time increment is the means of translating the discrete characteristics into analog characteristics. The smaller the time increment, the closer the discrete model approaches the analog process. The smaller the time increment, however, the greater the computer time necessary to simulate a given time period. Thus, a compromise between minimizing the departure from analog characteristics and realistic computer execution time is necessary.

SCHEDULED PARAMETER ADJUSTMEENT (TIME=V)

The capability to schedule a change in one or more parameters at a specified time greatly increases the flexibility of batch DynaChem executions. Reference Table 2 shows the Specification Keywords for which this capability applies.

Unit and Node State may not be adjusted using (TIME=v) and, in general, equipment changes are not allowed. 'Me following briefly summarize the types of parameters for which (TIME=v) is NOT allowed:

1) Unit Geometry - CSA, Volume, Height, Length, Exit Level
2) Controller algorithm and capabilities -NOWINDUP
3) Valve type, capacity, Rangeability, Pressure function
4) Pump curves, elevation, suction pressure drop

Many of these, including most equipment changes, may be altered in the Interactive Mode of DynaChem (See =INTERACTIVE Capability). For example, in Interactive Mode, a Tank size, exit level and valve capacity may be altered by Interrupting Execution and making the changes using the supplied Screens.

The parameters which may be adjusted with Scheduled Parameter. Adjustment (TIME=v) are summarized as follows-.

1) Controller Settings (Primary Keyword CLOOP)

CFACTOR=v	Controller output factor
CLOSE=v	Switch algorithm Close setpoint
DEADTIME=v	Dead Time
KC=v	Gain
OLIMIT=vl,v2	Controller output limits
OPEN=v	Switch algorithm Open setpoint
RATIO=v	Ratio Controller ratio value (see note)
SPVAL=vl,v2	Setpoint value(s)
TAUD=v	Integral time
TAUI=v	Derivative time
TRIM=vl,v2	Trim controller limits (see notes)
VCONSTANT=v	Valve constant (Bias)

Note: RATIO and TRIM may be used to adjust the associated numerical values only if the algorithm in effect already (i.e., at TIME=0).

2) Valve Position (Primary Keyword VALVE)

VOPEN=V	Valve override

3) Pump Switch (Primary Keyword PUMP)

PSWITCH=V	Pump speed override

4) Pipe temperature (Primary Keyword UNM

TDISCHARGE=V	Pipe discharge temperature
TMAX=V	Pipe maximum temperature
TMIN=V	Pipe minimum temperature

5) Time Increment (Primary Keyword TIME)

TINC=V	Time increment

6) Unit Equilibrium Computation (Primary Keyword UNIT)

	NOEQ	Do not compute equilibrium after specified time (conserve mass and energy, estimate temperature, pH, etc.)
	NOVAP	Do not allow vapor after specified time
7)	Output (Primary Keyword PRINT)	
	NOTERM	No output to Terminal
	OUTPUT=v	Output file (.DOU) frequency
	SUMMARY=v	Summary file (.SUM frequency
	TERM	Output to Terminal
	TRACE=v	Trace file (.OUE) frequency
8)	Output to Restart File (Primary Keyword SAVE)	
	FREQUENCY=v	Frequency of saving Restart (.ROU file)

Chapter 9: PRINT SPECIFICATION

The PRINT Keyword is used to specify the frequency of printing Output, Summary and Trace files to the Disk. Frequency is in terms of number of time increments.

The standard Terminal output (TRACE) is very brief, merely printing the current accumulated time. If, however, that is to be suppressed as well, NOTERM may be used.

The Interactive capabilities of DynaChem are invoked using the INTERACTIVE Specification. This automatically suppresses all normal terminal output and shifts the User into the screen driven Interactive process. Virtually all operating and Specification parameters may be changed dynamically while in the Interactive mode.

PRINT

Specifications (Optional):

OUTPUT=n	Output (File .DOU) Frequency in Number of Time Increments (default=10) For example, OUTPUT=0 for no output to .DOU file; OUTPUT=1 for output to .DOU file each time increment; OUTPUT= 10 for output to .DOU file on 1st, 10th, 20th, ... time increment.
SUMMARY=n	Summary (File .SUM) Frequency in Number of Time Increments (default=1)
TRACE=n	Trace (Fide .SUM) Frequency in Number of Time Increments (default=0)
NOTERM	No output to Terminal (default=Output to Terminal except when INTERACTIVE entered)
TERM	Output to Terminal (default=Output to Terminal except when INTERACTIVE entered)
INTERACTIVE	Interactive Mode and no output to the Terminal. (default=Output to Terminal).

The Output (.DOU) File begins with an echo of the Input. The OUTPUT specification designates the frequency with which the following information for a time increment is. written: For each. Unit and Node, the composition, enthalpy, density and volume for each phase (liquid, solid and vapor), temperature, pressure and liquid phase pH.

To the Summary (.SUM) File, is written at the specified frequency, a one-line summary for each Unit, Node and Valve/Control Loop.

Chapter 10: SAVE SPECIFICATION

The SAVE Keyword allows the User to save DynaChem information across two dimensions: space and time.

The Specification Keyword FREQUENCY allows the User to save the entire process (dimension: space) at a specified point in time. The Specification itself designates how often the entire process is to be saved. The resulting saved file may be used in a RESTART to initialize and restart the process at the time it was saved.

LOGNODE allows the User to save across the entire simulation time (dimension: time) a specified point in the process (a Node). The Specification designates the Node(s) to be saved. The resulting saved file may be used in an ENTRY Unit to enter the mass and energy at that Node as a scheduled inflow to the subsequent model. (See LOGNODE capability).

SAVE

Specifications (Optional):

FREQUENCY=v	Frequency of saving entire process to Restart File (hr) (default=at TEND only)
LOGNODE=nl,n2....	Nodes to be saved in the Node Output file for all time increments to be used, as input in an ENTRY Unit in a subsequent ran.

LOGNODE CAPABILITY

The LOGNODE capability allows the user to save, for all time steps, the State (temperature, pressure, flow and composition) of up to 10 Nodes. A subsequent execution may then use the saved information in an ENTRY Unit as a Feed stream.

In the first execution, save the information at Nodes n1, n2.....

SAVE LOGNODE=ni,n2,...

A complete description of the Nodes, at all times computed, are- stored in the Node Output file. That Output file becomes the Node Input file for the second execution. In that execution, the Nodes stored in the above procedures may now be used as follows:

UNITi LOGNODE=n1 DNODE=m1

UNITj LOGNODE=n2 DNODE=m2

. . .

. . .

The values n1, n2, ... are not actually Node ID Numbers in this execution, therefore, they may be used elsewhere as Node Numbers. For example, it is legal, but not necessary, for m1=n1, m2=n2,..., which makes translation from the first to the second execution easier.

The LOGNODE capability allows the user to separate the process into sections. Each section may then be isolated and analyzed, saving significant execution time. For example, the feed streams of a neutralization process may be analyzed and the level control loop "tuned", resulting in a single feed stream to the first Neutralization Stage. The first Stage may then be isolated and tuned without recalculating the feed section or computing the second Neutralization Stage. The resulting output stream from the first Stage may then be used as a simple feed stream to the second Stage, eliminating the need to recompute the Feed and first Stage repetitively while tuning the second Stage.

Chapter 11: RESTART SPECIFICATION

RESTART has no associated Specification Keywords. When RESTART is invoked, the stored values for the Keywords: TRME, NODE, UNIT, VALVE and CLOOP are retrieved from the Restart Input (.RIN) file along with the final conditions of all Units and Nodes at the last time stored. Therefore, entries for these Keywords are unnecessary unless they are entered with (TIME=v), where v is a time greater than the time at which the information was stored.

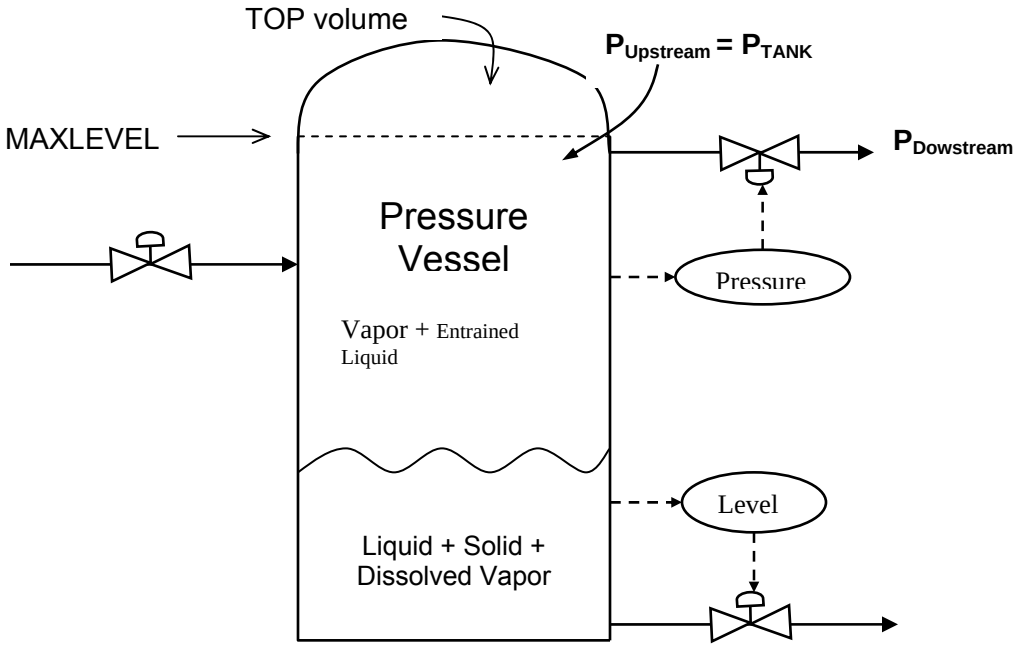
The execution begins at the last time stored. New entries for TIME, PRINT and SAVE must be entered for the RESTART execution if required. (See SAVE SPECIFICATION)

RESTART

Specifications:

None

Chapter 12: DynaChem Pressure Vessel



Use of the DynaChem Pressure Vessel

1) The Pressure Vessel is a TANK Unit with the Keyword "PV" included.

```
UNIT3    TANK   PV       UNODE=1   DNODE=3,10        "SURGE TANK"
         CSA=19.635     MAXL=10    LEXI=0.25,10
                  COND= TEMP 20.0    PRES 1.5TOTA  135    H2O  1.0   CO2  0.001
```

2) The Void volume in the TANK is computed as the volume above the liquid level including the TOP volume.

Void Volume (m^3) = (MAXLEVEL – Liquid Level) (m) * CSA (m^2) +
TOP Volume (m^3)

3) When the TANK has been specified as a Pressure Vessel, the top Exit must have a valve with a downstream pressure. The downstream pressure is specified in the VALV section with the Keyword "PDOWN."

VALV10 DNODE=10 CV=10 VOPEN=1.0 **PDOWN=1.0**

In this case, Downstream Node 10 from the above TANK (UNIT3) will have a valve with C_V = 10 m^3/hr and will begin in an Open position (VOPEN=1.0). The downstream pressure will be 1 atm (PDOWN=1.0).

4) The pressure in the Void Volume is computed after the TANK equilibrium computation. The equilibrium condition in the TANK is determined using an estimated pressure (P_{TANK}). With the equilibrium results including the vapor compressibility (z), temperature (T_K) and the moles of vapor ($Vapor_{moles}$), the pressure in the void space is determined:

P_{Void} (atm) = z ($Vapor_{moles}$) R T_K / Void Volume (m^3)

Based upon the P_{Void} and $P_{Downstream}$, the TANK pressure (P_{TANK}) is determined:

When $P_{Void} \leq P_{Downstream}$ then P_{TANK} is set equal to $P_{Downstream}$ and the equilibrium is recomputed. Under these conditions no flow may occur and the effective TANK pressure is the downstream pressure. Thus, $P_{TANK} = P_{Downstream}$ and the pressure difference across the valve is zero.

When $P_{Void} > P_{Downstream}$ then P_{TANK} is set equal to P_{Void} and the equilibrium is recomputed. This computation is done iteratively until the pressure used for the computation (P_{TANK}) is the same as the resulting computed Void Volume pressure (P_{Void}). Under these conditions, flow may occur depending upon the VALV computation.

5) In step 3 above, VALV10 is specified with a downstream pressure of 1 atm. Another necessary specification is the type of pressure function to be used in computing the flow through the valve. The Keyword used is “PFCN” as shown below:

VALV10 DNODE=10 CV=10 VOPEN=1.0 PDOWN=1.0 **PFCN=3**

The Pressure Function has four alternative forms. The form to be used is determined by the value entered for PFCN. The forms are as follows:

When PFCN = 0 (default), then

$$Pfactor = 1.0$$

When PFCN = 1, then

$$Pfactor = \left[P_{Upstream} - P_{Downtream}\right]^{1/2}$$

When PFCN = 2, then

$$Pfactor = \left[P_{Average}\left(P_{Upstream} - P_{Downtream}\right)\right]^{1/2}$$

$$\text{where } P_{Average} = \frac{\left(P_{Upstream} - P_{Downtream}\right)}{2}$$

When PFCN = 3, then

When $P_{Downstream}/P_{Upstream} \leq 0.53$ (subcritical flow)

$$Pfactor = P_{Upstream}(0.599625)$$

When $P_{Downstream}/P_{Upstream} > 0.53$ (critical flow)

$$Pfactor = P_{Upstream}\left[\frac{1-\left(P_{Downstream}/P_{Upstream}\right)^{2}}{2}\right]^{1/2}$$

6) The flow through the valve is then computed:

   Flow (m^3/hr) = Port * C_V * Pfac

7) The Port (Valve Port opening = Stem position) may be set manually or by a Control Loop. In VALV10 above, the Stem position is set at 1.0 (VOPEN=1.0) and will not change until another manual setting, such as

```
VALV10  DNODE=10      CV=10
        VOPEN=1.0 (TIME=0.0)          VOPEN=0.5 (TIME=0.5)
                PDOWN=1.0    PFCN=3
```

   where the Stem position is 1.0 from Time = 0.0 hour until Time = 0.5 hour, at which time the Stem position is changed to 0.5.

The Stem position may also be changed by a Control Loop. The following Control Loop controls VALV10 (VID=10). The Setpoint is the pressure (SPID=PRES) in UNIT3 (SPUN=3). The Setpoint value is 3 atm (SPVA=3.0). The PID control parameters include the Gain (KC=0.2) and the Integral time (TAUI =1.0).

```
CLOO2   VID=10 VELO   SPUN=3          SPID=PRES     SPVA=3.0 (TIME=0)
        TAUI =1.0     KC=0.2 (TIME=0)
```

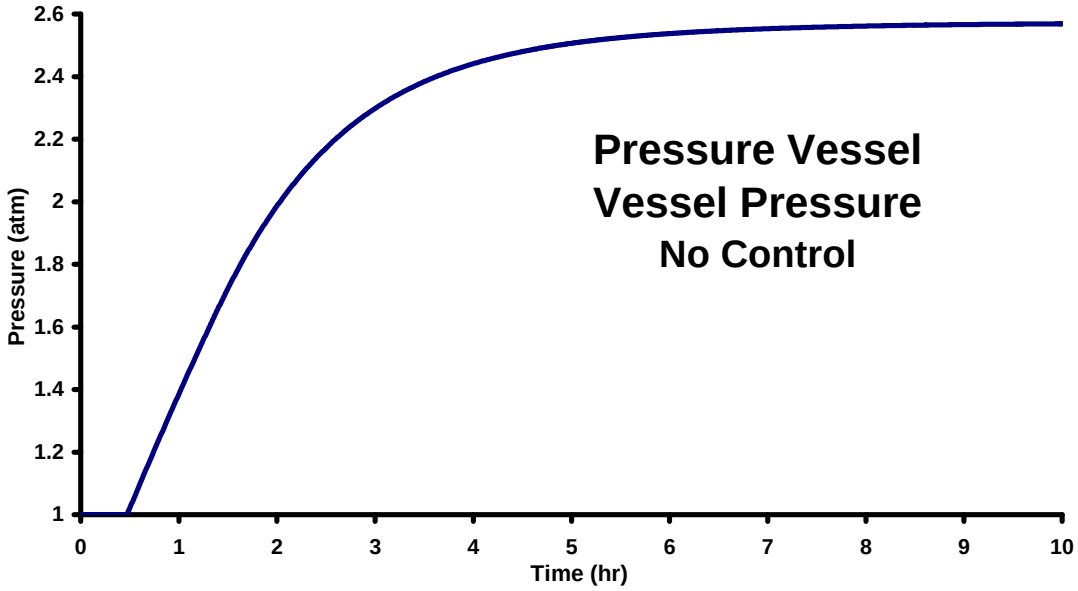
The Control loop will adjust the Stem position on VALV10 to result in a pressure of 3 atm in the TANK.

Example of a Single DynaChem Pressure Vessel

The above Pressure Vessel was initiated with 135 m^3 of H_2O with a small amount of dissolved CO_2 (0.1 % molar). A stream is fed to the vessel at a rate of 120 m^3/hr. The composition of the feed in molar percent is

H_2O	98.4% molar
HNO_3	1.24%
H_2SO_4	0.18%
$NANO_3$	0.018%
NA_2CO_3	0.007%
CO_2	0.18%

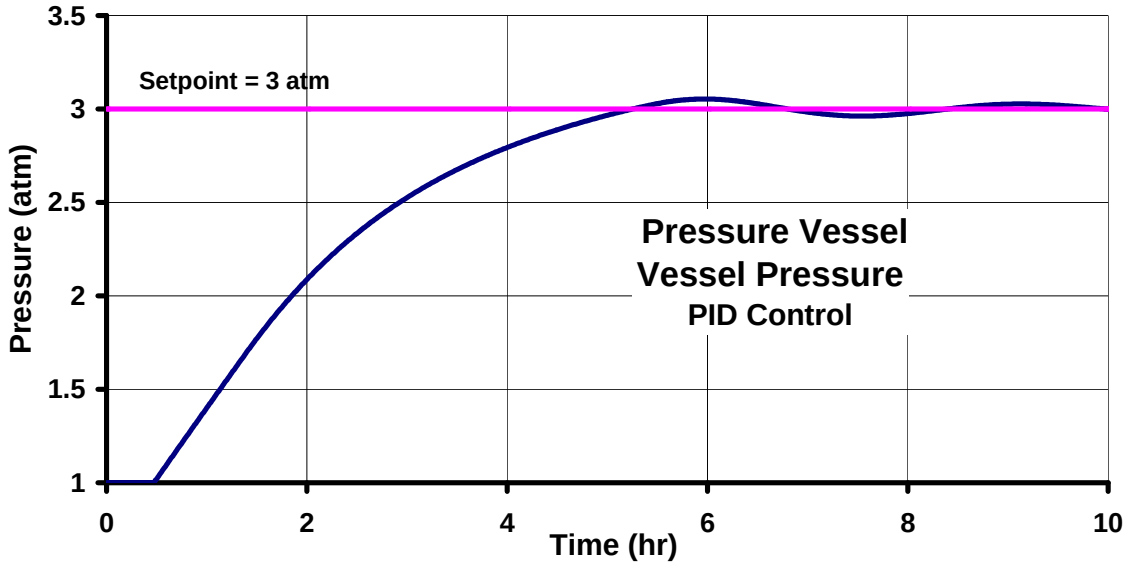
The result is a relatively slow evolution of vapor, which is predominately CO_2 and H_2O. With the downstream pressure of 1.0 atm and the Stem position permanently set to 1.0, the vessel builds up pressure from Time = 0.0 until it reaches the downstream pressure at Time = 0.48 hour. At that time, the pressure continues to increase above the downstream pressure and vapor begins to flow.



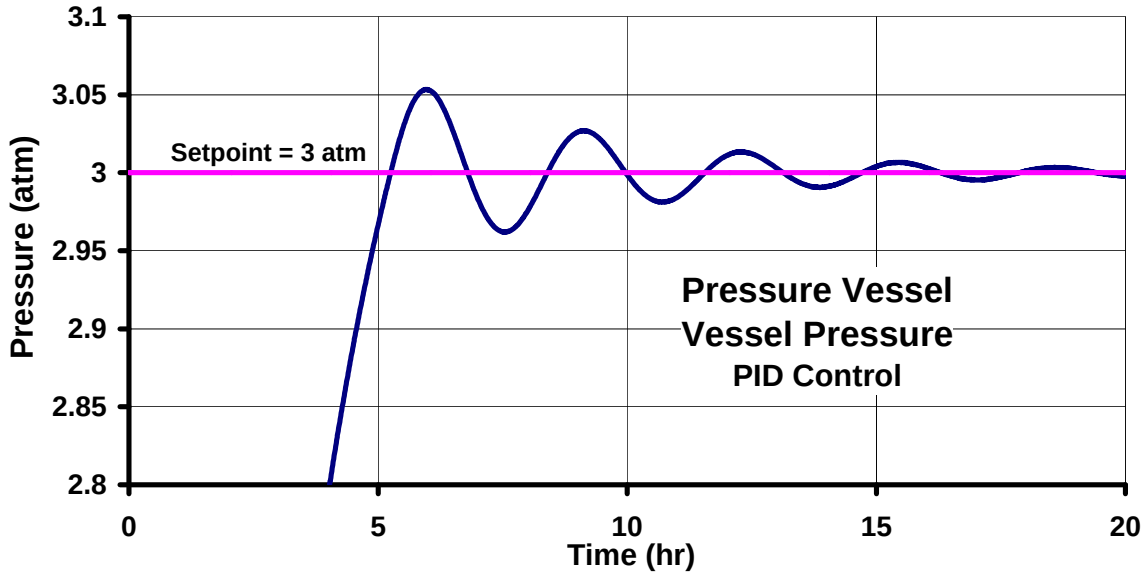
The pressure in the vessel begins to "level off" and come to steady state when the pressure in the vessel is sufficient to result in equilibration of the flow out through the valve and the vapor evolved from the solution in the tank. In this case, the steady-state pressure is 2.57 atm and has essentially reached that point after 6 hours.

Thus, with the valve 100% open, the pressure equilibrates to 2.57 atm. If, however, one wishes to control the pressure to 3 atm, there is a Stem position between 0 and 100% that should result in the increase pressure.

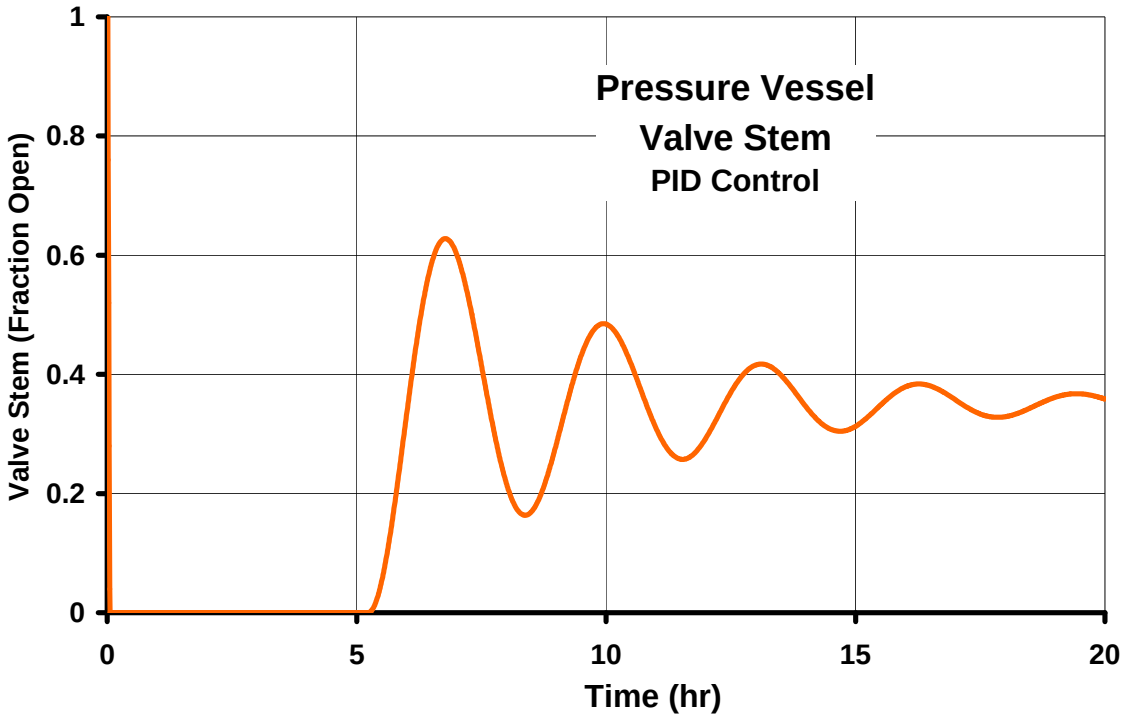
The Control Loop described in step 7 above results in the following response:



Magnification of the Time after 4 hours is as follows:



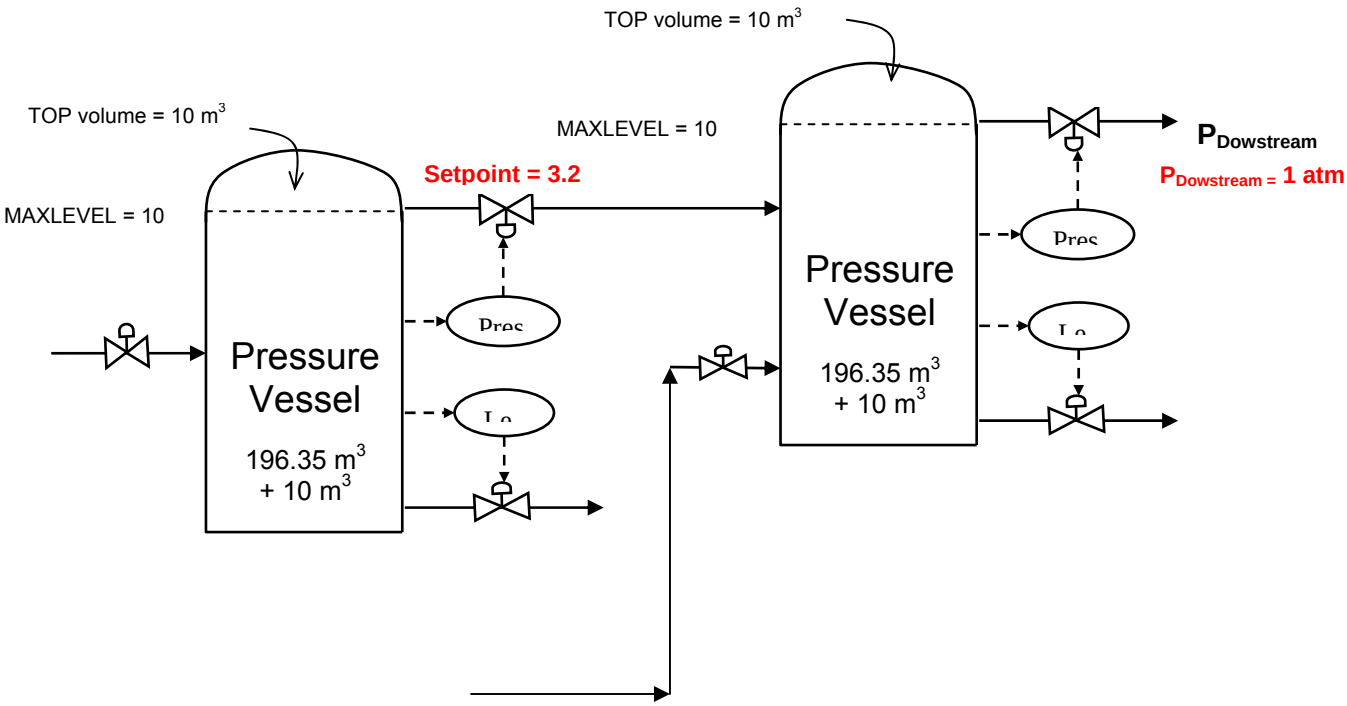
The Stem movement resulting in the above response is as follows:



Note that the valve remains closed until a little past 5 hours at which time the Void space has accumulated enough vapor to result in a Void volume pressure of 3 atm. It is then that the PID controller begins adjusting the Stem position based upon the Control Setpoint and Measured value.

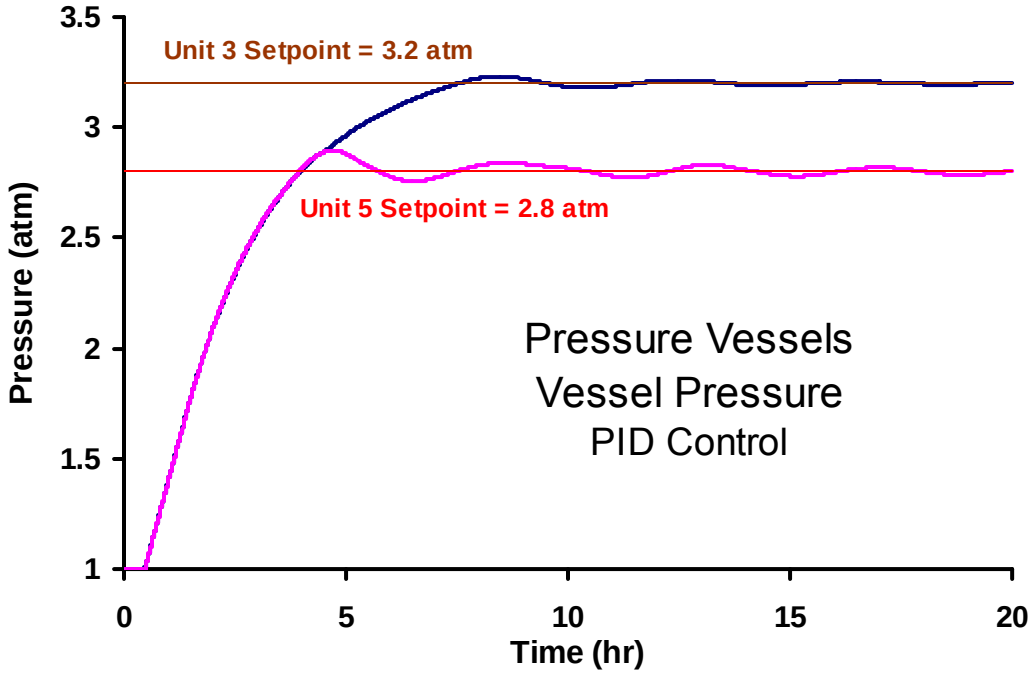
Example of Consecutive DynaChem Pressure Vessels

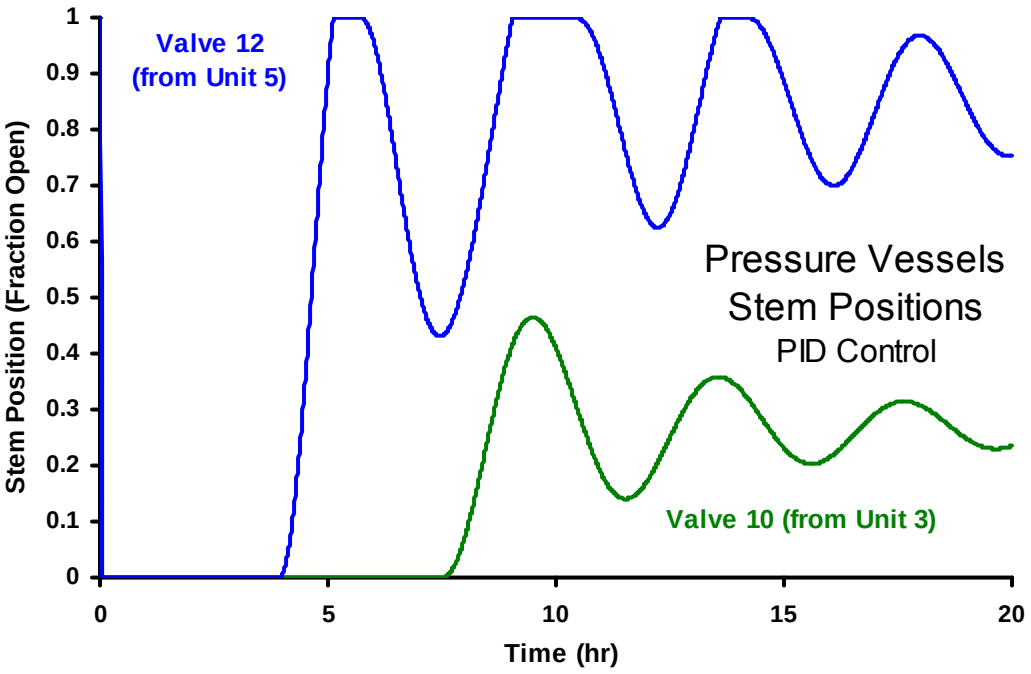
The following describes two consecutive DynaChem Pressure Vessels. The downstream pressure of the first vessel (Unit 3) is the pressure of the second vessel (Unit 5). The downstream pressure of the second vessel (Unit 5) is set by the valve on its vapor exit ($P_{Downstream}$). Both vessels are initiated with the same contents as in the above single-vessel case and both were fed with the same stream as above single-vessel case. The vessel geometries (i.e., CSA, Maximum Level, Exit Levels) and Control Loop parameters are also the same as in the single-vessel case.

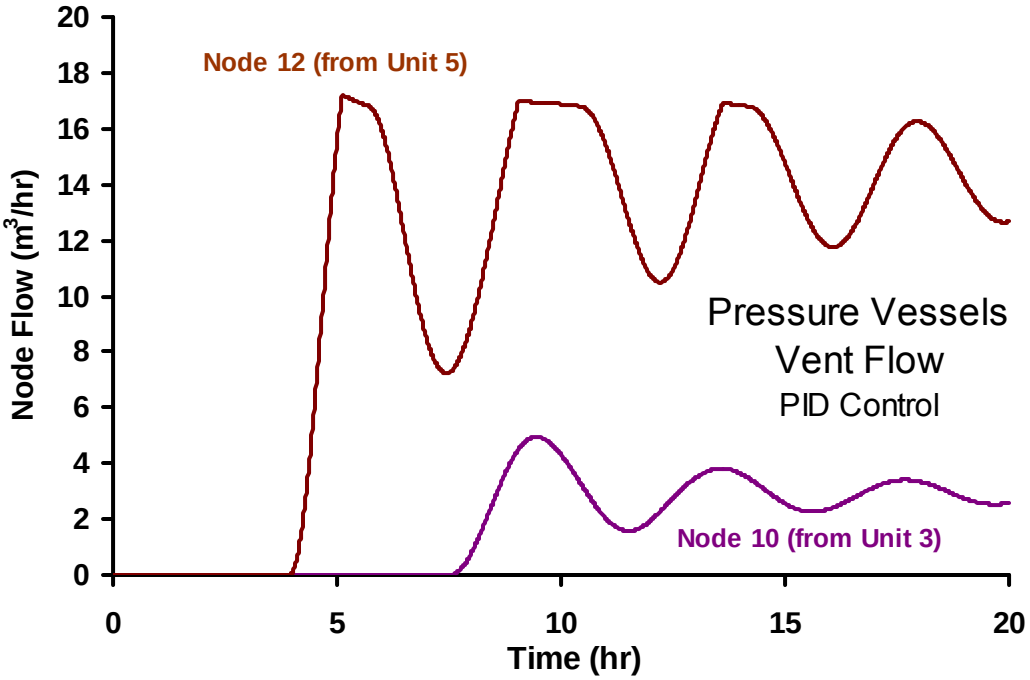


The control loops were set to control the pressure of the upstream vessel (Unit 3) at **3.2 atm** and the downstream vessel (Unit 5) at **2.8 atm**. The value for $P_{Dowstream}$ was set at **1 atm**.

As in the single-vessel case, the result is a relatively slow evolution of vapor in both vessels, which is predominately CO_2 and H_2O. The pressure begins to increase in each vessel with the vapor outlet valves closed and vapor accumulating in each vessel. When the downstream vessel (Unit 5) approaches its setpoint (2.8 atm), the valve opens and begins releasing vapor to equilibrate the pressure at the setpoint. Meanwhile, the vapor outlet valve on the upstream vessel (Unit 3) remains closed until its pressure reaches its setpoint (3.2 atm). After that, the controllers on the vapor outlet valves on each vessel adjust the valve stem position to achieve the desired setpoint pressure.


Unit 3 Setpoint = 3.2 atm
Unit 5 Setpoint = 2.8 atm
Pressure Vessels
Vessel Pressure
PID Control
Pressure (atm)
Time (hr)
3.5
3
2.5
2
1.5
1
0
5
10
15
20


Valve 12
(from Unit 5)
Valve 10 (from Unit 3)
Pressure Vessels
Stem Positions
PID Control
Stem Position (Fraction Open)
Time (hr)
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
5
10
15
20



From the dampening of the oscillations in the flow through the two vapor outlet valves, it is apparent that both vessels are approaching steady state after 20 hours. There are, perhaps, better combinations of Valve Capacity (C_V), PID Gain (K_C), PID Integral time (Taul), or other process parameters which would achieve a faster approach to steady state.

Another valuable exercise would be to perturb the process with increased feed flow, different feed composition, different pressure setpoints, etc., to determine the response. So far nothing has been said about the liquid level control. That could become an issue if the feed flow is substantially increased. Level settings on the liquid level Deadband control may not be achievable if the flow increases. The liquid valve may need to be increased in size or another control scheme devised. All of these and many other scenarios can be tested with the DynaChem model.

DynaChem Input Files

CASE: Single DynaChem Pressure Vessel

```
TITLE TWO CONSECUTIVE PRESSURE VESSELS WITHOUT CONTROL
;
PRINT OUTPUT=1  SUMMARY=1  INTERA
;
TIME   TEND=20.   TINC=.01 (TIME=0) TITLE TWO-STAGE NEUTRALIZATION
;
UNIT1  ENTRY  DNODE=1  "CONTINUOUS FEED"
   COND=TEMP 30.0   PRES 2.0  TOTA  120.0
+    H2O 55.51  HNO3 0.7   H2SO4 0.1  NANO3 0.01
+    NA2CO3 0.004   CO2 0.1
;
UNIT3  TANK  PV  TOP=10
   UNODE=1     DNODE=3,10  "SURGE TANK 1"  CSA=19.635  MAXL=10
   LEXI=.25,10
   COND= TEMP 20.0  PRES 1  TOTA  135  H2O  1.0  CO2  0.001
;
UNIT4  ENTRY  DNODE=9  "CONTINUOUS FEED 2"
   COND=TEMP 30.0   PRES 2.0  TOTA  120.0
+    H2O 55.51  HNO3 0.7   H2SO4 0.1  NANO3 0.01
+    NA2CO3 0.004   CO2 0.1
;
UNIT5  TANK  PV  TOP=10
   UNODE=9,10     DNODE=4,12  "SURGE TANK 2"  CSA=19.635  MAXL=10
   LEXI=.25,10
   COND= TEMP 20.0  PRES 1.5  TOTA  135  H2O  1.0  CO2  0.001
;
VALV1  DNODE=1  CV=100  VOPE=1 (TIME=0)
;
VALV2  DNODE=9  CV=100  VOPE=1 (TIME=0)
;
VALV3  DNODE=3  CV=100
;
VALV4  DNODE=4  CV=100
;
VALV10  DNODE=10  CV=10  VOPE=1.0  PFCN=3
;
VALV12  DNODE=12  CV=10  VOPE=1.0  PFCN=3  PDOWN=1.0
;
CLOO1  VID=3  POSI  SPUN=3  SPID=LEVEL  SPVA=2,7 (TIME=0)
   KC=.2 (TIME=0)  VCON=.35 (TIME=0)
;
CLOO4  VID=4  POSI  SPUN=3  SPID=LEVEL  SPVA=2,7 (TIME=0)
   KC=.2 (TIME=0)  VCON=.35 (TIME=0)
;
NODE ORDER=1,9,3,4
```

CASE: Consecutive DynaChem Pressure Vessels

```
TITLE TWO CONSECUTIVE PRESSURE VESSELS WITH CONTROL
;
PRINT OUTPUT=1  SUMMARY=1  INTERA
;
TIME   TEND=20.   TINC=.01 (TIME=0)
;
UNIT1  ENTRY  DNODE=1  "CONTINUOUS FEED"
   COND=TEMP 30.0   PRES 2.0  TOTA  120.0
+    H2O 55.51  HNO3 0.7   H2SO4 0.1  NANO3 0.01
+    NA2CO3 0.004   CO2 0.1
;
UNIT3  TANK  PV  TOP=10
   UNODE=1     DNODE=3,10  "SURGE TANK 1"  CSA=19.635  MAXL=10
   LEXI=.25,10
   COND= TEMP 20.0  PRES 1  TOTA  135  H2O  1.0  CO2  0.001
;
UNIT4  ENTRY  DNODE=9  "CONTINUOUS FEED 2"
   COND=TEMP 30.0   PRES 2.0  TOTA  120.0
+    H2O 55.51  HNO3 0.7   H2SO4 0.1  NANO3 0.01
+    NA2CO3 0.004   CO2 0.1
;
UNIT5  TANK  PV  TOP=10
   UNODE=9,10     DNODE=4,12  "SURGE TANK 2"  CSA=19.635  MAXL=10
   LEXI=.25,10
   COND= TEMP 20.0  PRES 1.5  TOTA  135  H2O  1.0  CO2  0.001
;
VALV1  DNODE=1  CV=100  VOPE=1 (TIME=0)
;
VALV2  DNODE=9  CV=100  VOPE=1 (TIME=0)
;
VALV3  DNODE=3  CV=100
;
VALV4  DNODE=4  CV=100
;
VALV10  DNODE=10  CV=10  VOPE=1.0  PFCN=3
;
VALV12  DNODE=12  CV=10  VOPE=1.0  PFCN=3  PDOWN=1.0
;
CLOO1  VID=3  POSI  SPUN=3  SPID=LEVEL  SPVA=2,7 (TIME=0)
   KC=.2 (TIME=0)  VCON=.35 (TIME=0)
;
CLOO4  VID=4  POSI  SPUN=3  SPID=LEVEL  SPVA=2,7 (TIME=0)
   KC=.2 (TIME=0)  VCON=.35 (TIME=0)
;
CLOO2  VID=10  VELO  SPUN=3  SPID=PRES  SPVA=3.2 (TIME=0)  TAUI =1.0
    KC=.2 (TIME=0)
;
CLOO3  VID=12  VELO  SPUN=5  SPID=PRES  SPVA=2.8 (TIME=0)  TAUI =1.0
    KC=.2 (TIME=0)
;
```

NODE ORDER=1,9,3,4

Chapter 13: CASE STUDIIES

The following cases are examples of the application of DynaChem to common engineering problems.

The first Example Case is a Five-Stage Ammonia Stripper which begins with pure water at 25 °C on all stages. Liquid containing water, ammonia and carbon dioxide is fed to the top of the column and steam is fed to the bottom. Two control schemes are tested. First (Case 1), the overhead vapor flow rate is controlled by adjusting the steam feed flow rate. Second (Case 1A), the bottoms ammonia composition is controlled by adjusting the steam feed flow rate. In both cases, the column reaches steady-state operation in 0.20 hour.

The second Example Case is a Two-Stage Neutralization of an aqueous stream containing sulfuric and nitric acids. The neutralization is being achieved with 20% NAOH in Stage 1 and 1% NAOH in Stage 2. Both NAOH flows are controlled by pH PID controllers with setpoints of 3 for the first stage and 9 for the second stage. One hour after startup the control stabilizes.

The third example is a tank with the initial contents at 90 °C and a continuous 95 °C feed. A cooling coil and recycle line are used to lower the temperature to 60 °C and maintain it at that level. The control scheme achieves the setpoint and stabilizes after 2.5 hours.

Case 1 - Five Stage Ammonia Stripper - Control Overhead Vapor Rate

Column Description

Five Stages with Stream Upflow through Liquid and Liquid Overflow

Stage Description:

Max Liq Level0.0883m

CSA - 0.318 m^2

Stage Capacity 0.028 m^3

Valve Description:

Feed Stream Valve	12	m^3	LINE Valve Override = 1
Fixed Steam Valve	1900	m^3	LINE Valve Override = 1
Trim Steam Valve	100	m^3	LINE Valve Override = 0

Initial Conditions

Liquid on Stages:

All Stages - Pure H_20

m^3

25°C

Operating Conditions

Liquid Feed: Begins at Time = 0

Temperature 43.333°C

Pressure 3.7415 atm

Total Flow 11.203 m^3/hr

H2O 0.91856 mole frac

NH3 0.06917

CO2 0.01227

Fixed Steam: Begins at Time = 0.015 hour (0.9 min)

Temperature 143°C

Pressure 3.7415 atm

Total Flow 1.8473E+03 m^3/hr

H2O 1.0 mole frac

Trim Steam: Valve Initially Closed

Temperature 143°C

Pressure 3.7415 atm

Total Flow 100 m^3/hr

H2O 1.0 mole frac

Control Loop Description:

Control Loop 1

Control Valve 13

Algorithm VELO

Setpoint Value 792.719

Value Type FLOW

Setpoint Node ID 6

Controller Gain -1.0E-04

Integral Tune 0.02

Calculation Order:

NODE ORDER=1,7,13,8,9,10,11,12,2,3,4,5,6

Approach to Equilibrium After 30 Minutes

Vapor Overhead (gmole/hr)	FraChem	DynaChem
H2O	45199	45198
NH3	41176	41175
CO2	7506	7506
Bottoms Liquid (gmole/hr)		
H2O	727881	727886
NH3	1225	1225
CO2	17.059	17.048
Temperature (°C)		
Stage 5	120.0	120.0
Stage 4	128.0	128.0
Stage 3	135.4	135.4
Stage 2	139.7	139.7
Stage I	141.1	141.1

Case 1A - Five Stage Ammonia Stripper - Control Bottoms Composition

Column Description:

Same as Example Case #1 except for Control Loop

Control Loop Description:

Control Loop 1

Control Valve 13

Algorithm VELO

Setpoint Value 2.00E-03

Value Type COMP

Setpoint Unit ID 1

Controller Gain	400
Integral Time	0.5
Species	NH3
Units	MOLF (.N4ole Fraction)
Phase	LIQ

Case 2 - Two Stage Neutralization

Operating Conditions

Continuous Feed:

Temperature	30°C
Pressure	1 atm
Total Flow	25 m^3/hr
H2O	55.51 relative
NANO3	0.01
H2SO4	0.1
HNO3	0.7
NA2CO	30.004

Intermittent Feed:

Begin Time = 0.5 hr, Duration = 0.25

Begin Time = 1.0 hr, Duration = 0.75

Begin Time = 2.25 hr, Duration = 0.5

Temperature	270°C
Pressure	1 atm
Total Flow	40 m^3/hr
H2O	55.51 relative
H2SO4	1.25
HNO3	0.15
NA2SO4	0.009

Buildup Feed:

Begin Time = 0.1 hr, Ramp Time = 0.35 hr, Duration = Continuous

Temperature 260°C

Pressure	1 atm	
Total Flow	10 m^3/hr	
H2O	55.51 relative	
NANO3	0.014	
HNO3	0.002	
NA2CO3	0.502	

Caustic Feed - 20% wt

Temperature	250°C	
Pressure	1 atm	
Total Flow	10 m^3/hr	
H2O	0.8988	
NAOH		0.1012

Caustic Feed - 1% wt

Temperature	25°C
Pressure	1 atm
Total Flow	60 m^3/hr
H20	0.9955
NAOH	4.52902E-03

Tank Description:

Surge Tank	CSA =19.635	Max Level = 10 m	Liquid Exit = 0.25 m
Stage 1	CSA =10	Max Level = 3 m	Liquid Exit = 3 m
Stage 2	CSA = 10	Max Level = 5 m	Liquid Exit = 0. 1, 5 m

Valve Description:

Valve	Downstream Node	Capacity m/hr	Type	Valve Override
1	1	100	LINE	1
2	2	100	LINE	1
3	3	100	LINE	
4	5	100	LINE	
5	7	20	LINE	
6	8	30	LINE	

Control Loop Description:

Loop	Valve	Unit	Algorithm	Type	Setpoint	Gain	Integral Time
1	3	3	POSI	Level	2, 4	0.2	(Valve Constant 0.35)
2	5	4	VELO	pH	3	-0.1	1
3	6	5	VELO	pH	9	-0.02	1
4	4	5	VELO	Level	4	0.15	2

Initial Conditions:

All Tanks: 20°C

1 Atm

Pure H2O

Surge Tank 35.3 m^3

Stage 127.0 m^3

Stage 249 0 m^3

NODE ORDER=1,2,9,10,3,7,4,8,5,6